**Supporting Information**

# Dissection of Alkylpyridinium Structures to Understand Deamination Reactions

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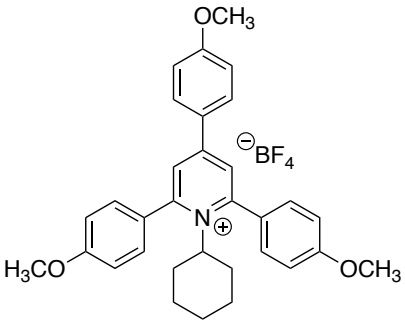
## General Information - Synthesis

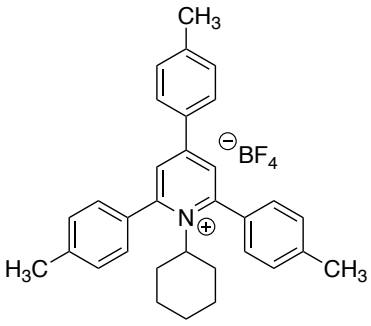
Reactions were performed in oven-dried Schlenk flasks or in oven-dried round-bottomed flasks unless otherwise noted. Round-bottomed flasks were fitted with rubber septa, and reactions were conducted under a positive pressure of $N_2$. Stainless steel syringes were used to transfer air- and moisture-sensitive liquids. Silica gel chromatography was performed on silica gel 60 (40-63 μm, 60Å) unless otherwise noted. Commercial reagents were purchased from Sigma Aldrich, Acros, Fisher, Strem, TCI, Combi Blocks, Alfa Aesar, AK Scientific, Oakwood, or Cambridge Isotopes Laboratories and used as received with the following exceptions: $CH_2Cl_2$ was dried by passing through drying columns.[1] Powdered, activated 4Å molecular sieves were prepared by heating sieves to ~200°C under high vacuum overnight and then crushing to achieve a fine powder. In some instances, oven-dried potassium carbonate was added to $CDCl_3$ to remove trace acid. Proton nuclear magnetic resonance ($^1$H NMR) spectra, carbon nuclear magnetic resonance ($^{13}$C NMR) spectra, and fluorine nuclear magnetic resonance spectra ($^{19}$F NMR) were recorded on both 400 MHz and 600 MHz spectrometers. Chemical shifts for protons are reported in parts per million downfield from tetramethylsilane and are referenced to residual protium in the NMR solvent ($CHCl_3$ = δ 7.26). Chemical shifts for carbon are reported in parts per million downfield from tetramethylsilane and are referenced to the carbon resonances of the solvent ($CDCl_3$ = δ 77.16). Chemical shifts for fluorine were externally referenced to $CFCl_3$ in $CDCl_3$ ($CFCl_3$ = δ 0). Data are represented as follows: chemical shift, multiplicity (br = broad, s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, m = multiplet, dd = doublet of doublets), coupling constants in Hertz (Hz), integration. Infrared (IR) spectra were obtained using FTIR spectrophotometers with material loaded onto a KBr plate. The mass spectral data were obtained at the University of Delaware mass spectrometry facility. Melting points were taken on a Thomas-Hoover Uni-Melt Capillary Melting Point Apparatus.

## Preparation of Alkylpyridinium Tetrafluoroborate Salts

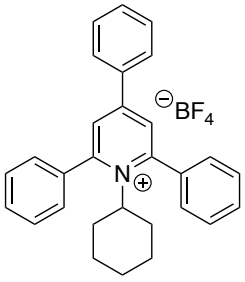
Pyridinium salts **1c-Cy** and **1c-i-Pr** were synthesized as described previously.[2] Pyridinium salts **1b-Cy** and **1d-Cy–1g-Cy** were synthesized according to General Procedure A. Pyridinium salts **1a-Cy** and **1n-Cy** were prepared as described below.



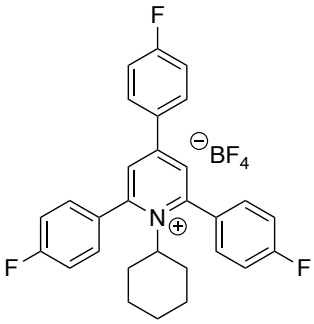

**1a-Cy**




**1b-Cy**




**1c-Cy**

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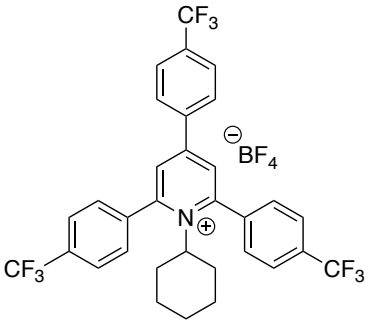
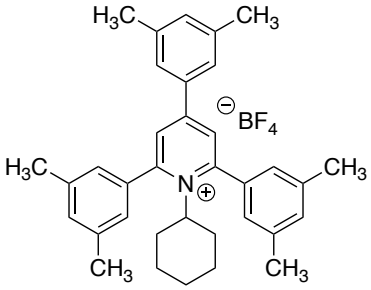
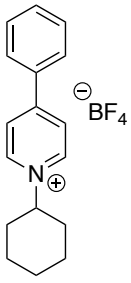


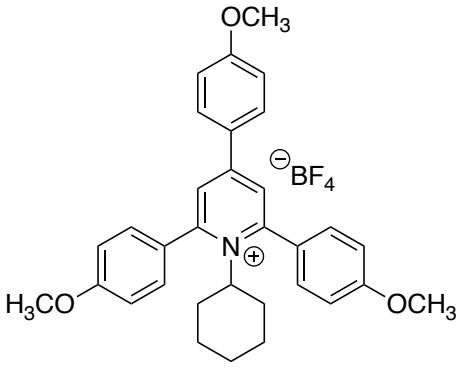

**1e-Cy**




**1g-Cy**




**1n-Cy**

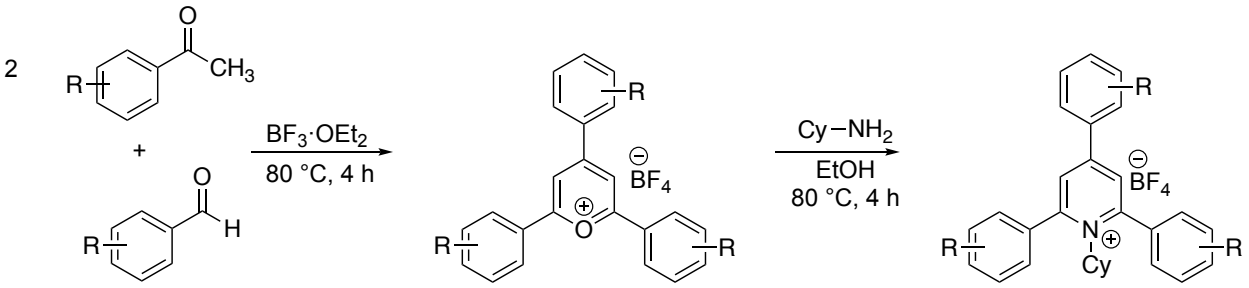


**1a-Cy**

**1-Cyclohexyl-2,4,6-tris(4-methoxyphenyl)pyridin-1-ium tetrafluoroborate (1a-Cy).** This procedure was adapted from Mouradzadegun and coworkers.[3] Under air, an oven-dried, round-bottomed flask was charged with a stir bar, 4-methoxybenzaldehyde (4.08 g, 30.0 mmol, 1.0 equiv), and 4'-methoxyacetophenone (9.01 g, 60.0 mmol, 2.0 equiv). As the solution was stirred, $POCl_3$ (25.0 mL, 270 mmol, 9.0 equiv) was added dropwise over 15 minutes, and the solution was then stirred at room temperature for an additional 15 minutes. A reflux condenser capped with a septum and a vent needle was attached, and the solution was then heated at 65 °C for 2 h. Then ethanol (30.0 mL, 1.0 M) and tetrafluoroboric acid (6.1 mL, 45.0 mmol, 1.5 equiv) were added sequentially. The mixture was then allowed to cool to room temperature and stirred at room temperature overnight. The product was precipitated by addition of $Et_2O$ (150 mL, ~5 times the mmol of aldehyde used). The resulting red solid pyrylium tetrafluoroborate salt was collected via filtration**,** washed with $Et_2O$ (3 x 25 mL), and dried under high vacuum to give the corresponding pyrylium salt (5.64 mg, 39%). The resulting pyrylium tetrafluoroborate salt was used directly without further purification.

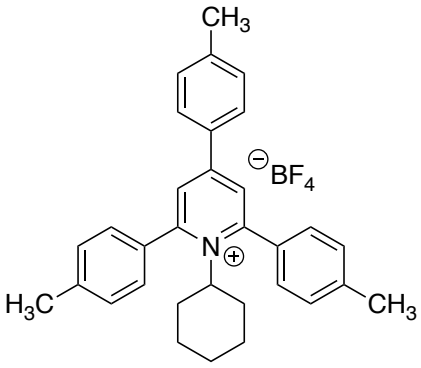
This procedure was adapted from our previous work.[2a] Under air, commercially available cyclohexyl amine (0.70 mL, 6.00 mmol, 1.2 equiv) was added to a suspension of tris(4-methoxyphenyl)pyrylium tetrafluoroborate salt (2.43 g, 5.00 mmol, 1.0 equiv) and EtOH (5.0 mL, 1.0 M) in a round-bottomed flask. The flask was fitted with a reflux condenser capped with a septum with a vent needle. The mixture was stirred and heated at reflux in an oil bath at 80–85 °C overnight. The mixture was then allowed to cool to room temperature. The crude mixture was purified by silica gel chromatography (1–10% $CH_3OH$ in $CH_2Cl_2$) to give desired product **1a** (1.75 g, 62%) as an orange-red powder (mp 115–117 °C): $^1$H NMR (600 MHz, $CDCl_3$) δ 7.85 – 7.80 (m, 4H), 7.75 – 7.70 (m, 4H), 7.14 – 7.11 (m, 4H), 7.06 – 7.02 (m, 2H), 4.70 – 4.59 (m, 1H), 3.94 (s, 6H), 3.90 (s, 3H), 2.15 (d, $J$ = 12.0 Hz, 2H), 1.67 – 1.60 (m, 2H), 1.60 – 1.50 (m, 2H), 1.41 (d, $J$ = 13.3 Hz, 1H), 0.92 – 0.80 (m, 2H), 0.76 – 0.64 (m, 1H); $^{13}$C NMR (151 MHz, $CDCl_3$) δ 163.4, 161.5, 157.4, 153.8, 131.3, 130.2, 126.9, 126.4, 125.8, 115.4, 114.4, 71.9, 55.8, 55.7, 34.1, 26.8, 24.9; $^{19}$F NMR (565 MHz, $CDCl_3$) δ –153.51 (minor, $^{11}BF_4$), –153.56 (major, $^{10}BF_4$); FTIR (neat) 2937, 1597, 1576, 1510, 1457, 1296, 1247, 1181, 1025, 836; HRMS (ESI+) $[M\text{-}BF_4]^+$ calculated for $C_{32}H_{34}NO_3$: 480.2533, found 480.2525.

## General Procedure A: Preparation of Pyridinium Tetrafluoroborate Salts




This procedure was adapted from Spokoyny and coworkers.[4] An oven-dried, round-bottomed flask was charged with a stir bar, the corresponding benzaldehyde (1.0 equiv), and the corresponding acetophenone (2.0 equiv). Toluene was used as solvent (1.0 M) for solid acetophenones. $BF_3 \cdot Et_2O$ (2.4 equiv) was added dropwise with stirring. The mixture was heated to 80 °C with a vent needle in the septum for 4 hours. The mixture was then allowed to cool to room temperature. The product was precipitated by addition of $Et_2O$ (mL = ~5 times the number of mmol of aldehyde used). The resulting solid pyrylium salt was collected via filtration and washed with $Et_2O$ (3 x 25 mL), dried under high vacuum, and used directly without any further purification.

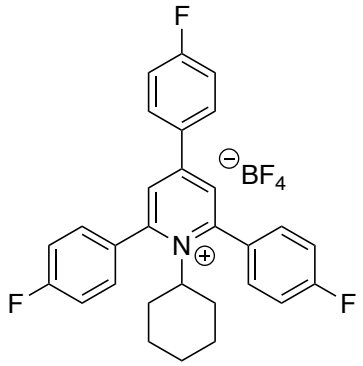
This procedure was adapted from our previous work.[5] Commercially available cyclohexyl amine (1.0 equiv) was added to a suspension of the corresponding pyrylium tetrafluoroborate (1.0 equiv), powdered activated 4Å molecular sieves (~500 mg/mmol), and $CH_2Cl_2$ (0.5 M) in a round-bottomed flask equipped with a stir bar. The flask was fitted with a septum and a vent needle. The mixture was stirred as $Et_3N$ (1.0 equiv for free base amines; 2.0 equiv for amine hydrochloride salts) was added by syringe. The vent needle was removed, and the mixture was stirred at rt for 30 min. The vent needle was reinserted before the addition of acetic acid (2.0 equiv). The needle was again removed, and the mixture was stirred at rt overnight. The mixture was then filtered through a short pad of Celite using $CH_2Cl_2$ to rinse the flask and Celite pad. The filtrate was then washed with distilled $H_2O$ (1 x 30 mL), and sat. NaCl (2 x 30 mL), dried ($NaSO_4$), filtered, and concentrated. $Et_2O$ (ca. 100 mL) was added to the solid to precipitate the pyridinium salt, which was then isolated by filtration. If the salt still did not precipitate, it was purified by silica gel chromatography with acetone/$CH_2Cl_2$ as the eluent.



**1b-Cy**

**1-Cyclohexyl-2,4,6-tri-*p*-tolylpyridin-1-ium tetrafluoroborate** (**1b-Cy).** Prepared via General Procedure A on a 20.0 mmol scale using the 4-methylbenzaldehyde (2.4 mL, 20.0 mmol, 1.0 equiv), 4-methylacetophenone (5.3 mL, 40.0 mmol, 2.0 equiv), and boron trifluoride diethyl etherate (5.9 mL, 48.0 mmol, 2.4 equiv) to give the corresponding pyrylium salt as a yellow solid (3.64 g, 8.31 mmol, 42%).

The pyrylium salt (2.0 mmol) was used directly without further purification to generate pyridinium salt **1b-Cy** following General Procedure A. The crude mixture was purified by silica gel chromatography (2–25% acetone in $CH_2Cl_2$) to give the desired product **1b-Cy** (482 mg, 0.928 mmol, 19%) as a light green crystalline solid (mp 131–136 °C): $^1$H NMR (600 MHz, $CDCl_3$) δ 7.76 (s, 2H), 7.65 (d, *J* = 8.2 Hz, 2H), 7.58 (d, *J* = 8.0 Hz, 4H), 7.37 (d, *J* = 7.9 Hz, 4H), 7.28 (d, *J* = 8.1 Hz, 2H), 4.66 – 4.58 (m, 1H), 2.48 (s, 6H), 2.39 (s, 3H), 2.08 (d, *J* = 11.7 Hz, 2H), 1.59 (d, *J* = 13.8 Hz, 2H), 1.56 – 1.47 (m, 2H), 1.36 (d, *J* = 13.1 Hz, 1H), 0.84 – 0.74 (m, 2H), 0.69 – 0.59 (m, 1H); $^{13}$C NMR (151 MHz, $CDCl_3$) δ 157.5, 154.7, 143.0, 141.3, 131.4, 131.2, 130.5, 129.6, 129.4, 128.3, 127.7, 71.8, 33.8, 26.6, 24.8, 21.7, 21.6;$^{19}$F NMR (565 MHz, $CDCl_3$) δ –153.60 (minor, $^{11}BF_4$), –153.66 (major, $^{10}BF_4$); FTIR (neat) 2932, 1620, 1559, 1512, 1140, 1056, 825, 732; HRMS (ESI+) $[M–BF_4]^+$ calculated for $C_{32}H_{34}N$: 432.2686, found 432.2689.

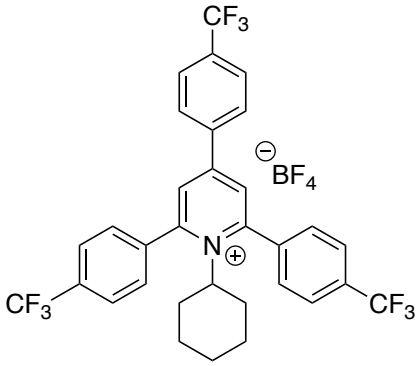


**1d-Cy**

**1-Cyclohexyl-2,4,6-tris(4-fluorophenyl)pyridin-1-ium tetrafluoroborate (1d-Cy).** Prepared via General Procedure A on a 10.0 mmol scale using the 4-fluorobenzaldehyde (1.1 mL, 10.0 mmol, 1.0 equiv), 4-fluoroacetophenone (2.4 mL, 20.0 mmol, 2.0 equiv) and boron trifluoride

diethyl etherate (3.0 mL, 24.0 mmol, 2.4 equiv) to give the corresponding pyrylium salt as a yellow solid (1.89 g, 4.19 mmol, 42%).

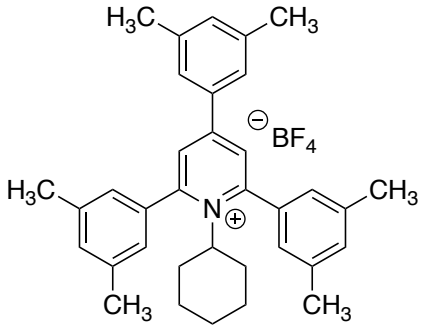
The pyrylium salt (2.0 mmol) was used directly without further purification to generate pyridinium salt **1d-Cy** following General Procedure A. The crude mixture was purified by silica gel chromatography (2–25% acetone in $CH_2Cl_2$) to give the desired product **1d-Cy** (284 mg, 0.535 mmol, 27%) as an orange powder (mp 126–130 °C): $^1$H NMR (600 MHz, $CDCl_3$) δ 7.80 – 7.70 (m, 8H), 7.30 – 7.23 (m, 4H), 7.19 – 7.12 (m, 2H), 4.61 – 4.49 (m, 1H), 2.11 (d, $J$ = 11.7 Hz, 2H), 1.61 (d, $J$ = 13.6 Hz, 2H), 1.49 – 1.36 (m, 3H), 0.86 – 0.73 (m, 2H), 0.72 – 0.60 (m, 1H); $^{13}$C NMR (151 MHz, $CDCl_3$) δ 165.3 (d, $J_{C–F}$ = 254.5 Hz), 164.1 (d, $J_{C–F}$ = 253.2 Hz), 156.5, 154.3, 131.8, 130.8, 130.7, 130.3 (d, $J_{C–F}$ = 3.2 Hz), 130.1 (d, $J_{C–F}$ = 3.7 Hz), 128.6, 117.1 (d, $J_{C–F}$ = 22.2 Hz), 116.3 (d, $J_{C–F}$ = 22.0 Hz). 72.2, 33.8, 26.7, 24.8; $^{19}$F NMR (565 MHz, $CDCl_3$) δ –106.79, –107.85, –152.85 (minor, $^{11}BF_4$), –152.90 (major, $^{10}BF_4$); FTIR (neat) 2935, 1622, 1601, 1509, 1236, 1163, 1140, 1055, 841, 545; HRMS (ESI+) $[M–BF_4]^+$ calculated for $C_{29}H_{25}F_3N$: 444.1934, found 444.1939.




**1e-Cy**

**1-Cyclohexyl-2,4,6-tris(4-(trifluoromethyl)phenyl)pyridin-1-ium tetrafluoroborate (1e-Cy).** Prepared via General Procedure A on a 20.0 mmol scale using the 4-trifluoromethylbenzaldehyde (2.7 mL, 20.0 mmol, 1.0 equiv), 4-trifluoromethylacetophenone (8.2 mL, 40.0 mmol, 2.0 equiv), and boron trifluoride diethyl etherate (5.9 mL, 48.0 mmol, 2.4 equiv) to give the corresponding pyrylium salt as a yellow solid (2.82 g, 4.70 mmol, 23%).

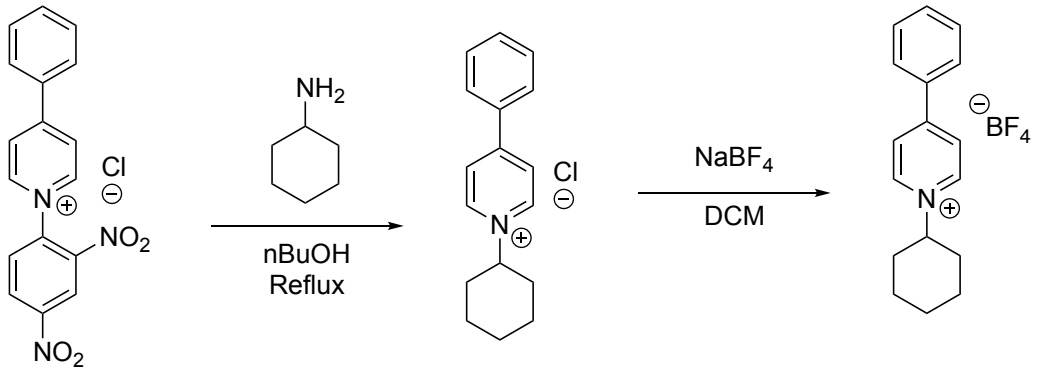
The pyrylium (2.0 mmol) was used directly without further purification following General Procedure A to give the desired product **1e** (1.34 g, 98%) as a white powder without purification (mp 177–179 °C): $^1$H NMR (600 MHz, $CDCl_3$) δ 7.93 (d, $J$ = 7.9 Hz, 4H), 7.82 (t, $J$ = 6.8 Hz, 6H), 7.76 (s, 2H), 7.66 (d, $J$ = 8.1 Hz, 2H), 4.60 – 4.44 (m, 1H), 2.18 (d, $J$ = 11.3 Hz, 2H), 1.60 (d, $J$ = 13.2 Hz, 2H), 1.47 – 1.34 (m, 3H), 0.81 – 0.69 (m, 2H), 0.67 – 0.57 (m, 1H); $^{13}$C NMR (151 MHz, $CDCl_3$) δ 156.1, 154.5, 137.7, 137.3, 133.4 (q, $J_{C–F}$ = 33.0 Hz), 130.3, 129.4, 129.0, 126.5 (q, $J_{C–F}$ = 3.7 Hz), 126.0, 123.6 (q, $J_{C–F}$ = 272.8 Hz), 123.5 (q, $J_{C–F}$ = 272.8 Hz), 73.0, 33.7, 26.6, 24.6; $^{19}$F NMR (565 MHz, $CDCl_3$) δ –63.09, –63.18, –152.36 (minor, $^{11}BF_4$), –152.41 (major, $^{10}BF_4$); FTIR (neat) 2941, 1628, 1615, 1566, 1409, 1324, 1172, 1131, 1055, 1020, 842, 733, 611; HRMS (ESI+) $[M–BF_4]^+$ calculated for $C_{32}H_{25}F_9N$: 594.1838, found 594.1825.



**1g-Cy**

**1-Cyclohexyl-2,4,6-tris(3,5-dimethylphenyl)pyridin-1-ium tetrafluoroborate (1g-Cy).** Prepared via General Procedure A on a 10.0 mmol scale using the 3,5-dimethylbenzaldehyde (1.3 mL, 10.0 mmol, 1.0 equiv), 3,5-dimethylacetophenone (3.0 mL, 20.0 mmol, 2.0 equiv), and boron trifluoride diethyl etherate (3.0 mL, 24.0 mmol, 2.4 equiv) to give the corresponding pyrylium salt as a yellow solid (1.47 g, 3.05 mmol, 31%).

The pyrylium salt (2.0 mmol) was used directly without further purification to generate pyridinium salt **1g-Cy** following General Procedure A. The crude mixture was purified by silica gel chromatography (2–25% acetone in $CH_2Cl_2$) to give the desired product **1g-Cy** (756 mg, 67%) as a white powder (mp 190–192 °C): $^1$H NMR (400 MHz, $CDCl_3$) δ 7.79 (s, 2H), 7.39 (s, 2H), 7.31 (s, 4H), 7.22 (s, 2H), 7.15 (s, 1H), 4.63 (dd, *J* = 13.4, 10.6 Hz, 1H), 2.43 (s, 12H), 2.36 (s, 6H), 2.11 (d, *J* = 11.9 Hz, 2H), 1.71 – 1.46 (m, 4H), 1.38 (d, *J* = 13.0 Hz, 1H), 0.88 – 0.74 (m, 2H), 0.73 – 0.63 (m, 1H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 157.5, 155.0, 139.5, 138.8, 134.1, 133.9, 133.8, 132.5, 127.7, 127.1, 126.1, 72.0, 34.0, 26.7, 24.9, 21.5, 21.4; $^{19}$F NMR (376 MHz, $CDCl_3$) δ –153.50 (minor, $^{11}BF_4$), –153.55 (major, $^{10}BF_4$); FTIR (neat) 2923, 1620, 1599, 1563, 1447, 1055, 851, 730, 711; HRMS (ESI+) $[M–BF_4]^+$ calculated for $C_{35}H_{40}N$: 474.3155, found 474.3151.



**S1** **S2** **1n-Cy**

**1-Cyclohexyl-4-phenyl-pyridin-1-ium tetrafluoroborate (1n-Cy).** 4-Phenyl Zincke salt **S1** was prepared according to literature procedure.[6] The procedure to generate 1-cyclohexyl-4-phenyl-pyridin-1-ium chloride (**S2**) was adapted from Castagnoli and coworkers.[7] Under air, a 50 mL, round-bottomed flask was charged with a stir bar and 4-phenyl Zincke salt **S1** (3.57 g, 10.0 mmol, 1.0 equiv). 1-Butanol (20 mL, 0.5 M) was added, followed by cyclohexyl amine (1.4 mL, 12.0 mmol, 1.2 equiv). A reflux condenser capped with a septum and vent needle

was attached, and the dark red solution was heated at 120 °C for 30 h. The mixture was then allowed to cool to room temperature. The product was precipitated with $Et_2O$ and stored in the freezer overnight to promote crystallization. The resulting tan solid was collected via filtration and washed with EtOAc until the filtrate was colorless. The solid was then washed with $Et_2O$ to remove EtOAc, collected, and dried under vacuum to give 1-cyclohexyl-4-phenyl-pyridin-1-ium chloride **S2** (2.65 g, 9.68 mmol, 97%) as a tan solid. Chloride **S2** was used without further purification.

To a separatory funnel was added 1-cyclohexyl-4-phenyl-pyridin-1-ium chloride **S2** (820 mg, 3.0 mmol, 1.0 equiv), and $CH_2Cl_2$ (50 mL). This mixture was washed with sat. aqueous sodium tetrafluoroborate (50 mL x 4) and then sat. aqueous sodium chloride (50 mL x 2), dried over $MgSO_4$, filtered, and concentrated under reduced pressure to give pyridinium salt **1n-Cy** (782 mg, 2.40 mmol, 80%) as a yellow solid (mp 130–132 °C): $^1$H NMR (400 MHz, $CDCl_3$) δ 8.92 (d, *J* = 6.2 Hz, 2H), 8.22 (d, *J* = 6.0 Hz, 2H), 7.83 – 7.74 (m, 2H), 7.61 – 7.49 (m, 2H), 4.66 – 4.51 (m, 1H), 2.22 (d, *J* = 11.3 Hz, 2H), 1.99 – 1.83 (m, 4H), 1.74 (d, *J* = 13.5 Hz, 1H), 1.60 – 1.46 (m, 2H), 1.37 – 1.21 (m, 1H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 156.9, 143.0, 133.7, 132.5, 130.1, 128.0, 125.5, 71.6, 33.7, 25.3, 24.5; $^{19}$F NMR (376 MHz, $CDCl_3$) δ –151.6 (minor, $^{11}BF_4$), –151.7 (major, $^{10}BF_4$); FTIR (neat) 2944, 2862, 1638, 1440, 1161, 1062, 854, 778, 729, 695; HRMS (ESI+) [M–$BF_4$]$^+$ calculated for $C_{17}H_{20}N$: 238.1596, found 238.1587.

## General Information – Electrochemistry

**Materials.** Tetrabutylammonium hexafluorophosphate ($TBAPF_6$) was purchased from Tokyo Chemical Industry Co. LTD, recrystallized from ethyl alcohol, and dried under vacuum at 40 °C for at least one week prior to use. Solvents for electrochemistry were of reagent grade or better and were dried by passage through activated alumina and then stored over 4 Å molecular sieves prior to use.

**Cyclic voltammetry (CV) and differential pulse voltammetry (DPV)** Experiments were performed using a CHI-620D potentiostat/galvanostat using a standard three-electrode configuration. The working electrode was a polished glassy carbon electrode (GCE, 3.0 mm diameter, CH Instruments) and the auxiliary electrode was a piece of platinum gauze. Electrochemical potentials were measured against a silver wire pseudo reference, unless otherwise noted, with an internal ferrocene standard. Reported electrochemistry data are calibrated and reported versus the $Fc/Fc^+$ couple. The supporting electrolyte employed for CV and DPV experiments was 0.1 M tetrabutylammonium hexafluorophosphate ($TBAPF_6$), dissolved in dry N,N-Dimethylformamide. The analyte concentration was 1.0 mM, and all CV experiments were carried out varying scan rates of $\nu$ = 5, 10, 25, 50, 75, 100, 250, 500, 750 and 1000 mV/s unless otherwise noted. For the scan rate experiments, data were collected from the fastest scan rate to the slowest scan rate. Before starting a new CV experiment, the solution was stirred at least 30 seconds to ensure complete homogeneity at the electrode/electrolyte interface and then allowed to rest for at least two minutes to ensure voltammetry was performed on quiescent solutions. All the CV and DPV experiments were performed under an inert atmosphere of $N_2$.

### *Voltammetric Simulations*

Electrochemical simulation of voltammetric traces were carried out using DigiElch (ElchSoft) software. Simulated voltammograms were fitted to experimental traces using a planar semi-infinite diffusion. For all simulations, the following parameters were applied: electrode area (A = 0.07 $cm^2$); temperature (T = 298 K); analyte concentration ([C] = 1.0 mM), diffusion coefficient (D = $10^{-5}$ $cm^2s^{-1}$); transfer coefficient ($\alpha$ = 0.5). Uncompensated resistance ($R_u$), with values ranging from 20 to 200 Ω, was obtained from experimental data and included in the simulation. An average double layer capacitance ($C_{dl}$ = 3 μF) was applied during the voltammetric simulation. Using all these input parameters, the experimental voltammograms were fitted to an EC mechanism involving a reversible electron transfer step followed by a chemical step, as follow:

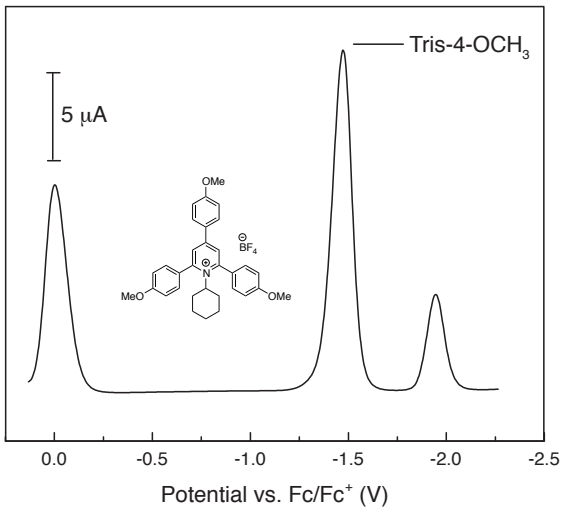
$$A + e^- \overset{ks,\ E^\circ}{\longleftrightarrow} B \xrightarrow{kf} C$$

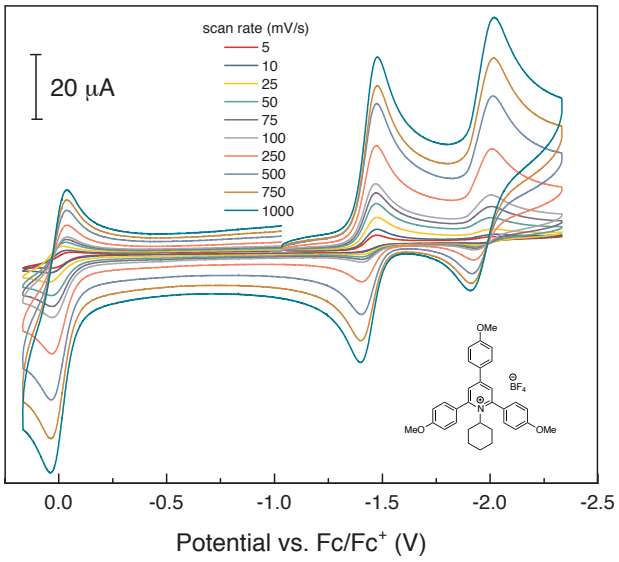
Using the implemented iterative non-linear least squares fitting algorithm, very good fittings were achieved for all experimental voltammograms. The fitting procedure was simultaneously applied to multiple voltammograms acquired at different scan rates. Optimal values for the output parameters, including the standard redox potentials ($E^\circ$), the heterogenous rate constant for SET ($k_s$), and the forward chemical rate constant ($k_f$) were obtained.

The values extracted from these simulations are shown in the table below, and are based on data displayed in the DPV and CVs of variable scan rate shown over the next 3 pages.

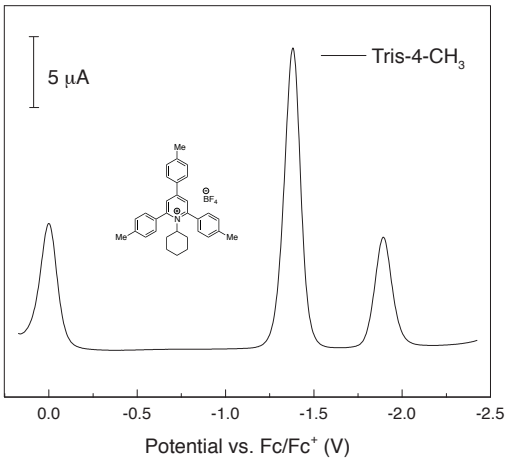
| Entry | Compound | $E°$ (V vs $Fc/Fc^+$) | $k_f$ ($s^{-1}$) |
|---|---|---|---|
| 1 | **1a-Cy** | –1.415 (± 0.003) | 0.39 (±0.04) |
| 2 | **1b-Cy** | –1.372 (± 0.005) | 0.20 (± 0.05) |
| 3 | **1c-Cy** | –1.341 (± 0.003) | 0.10 (± 0.04) |
| 4 | **1d-Cy** | –1.296 (± 0.007) | 0.17 (± 0.02) |
| 5 | **1e-Cy** | –1.102 (±0.005) | 0.07 (±0.06) |
| 6 | **1g-Cy** | –1.371 (± 0.010) | 0.13 (± 0.04) |

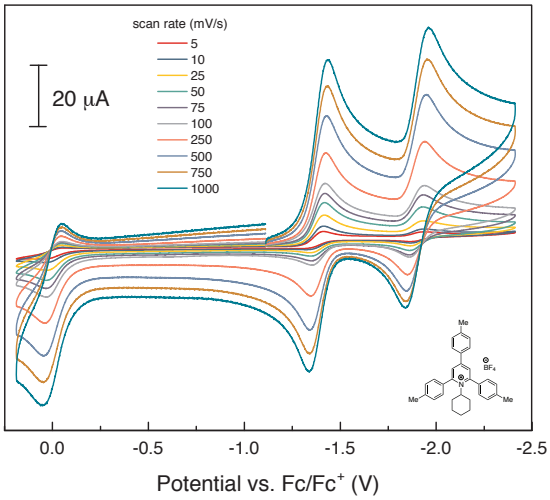
**1a-Cy**



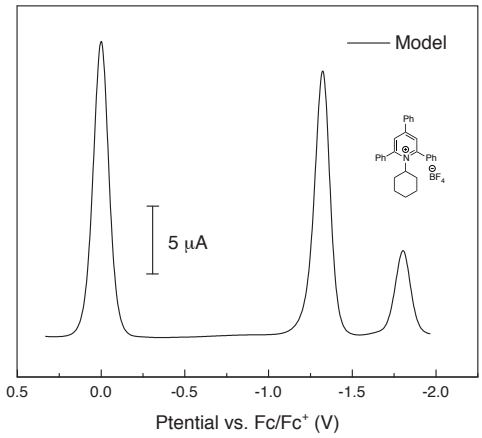



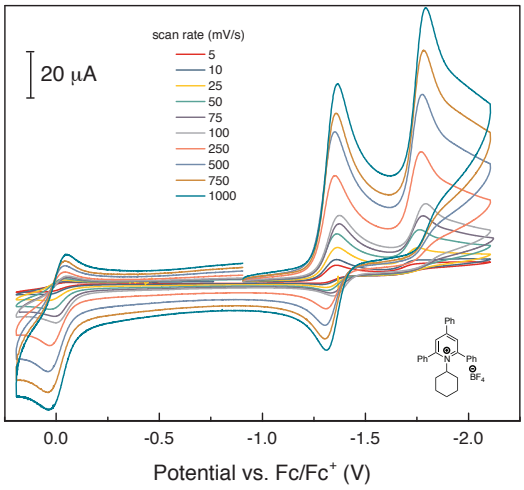

**1b-Cy**



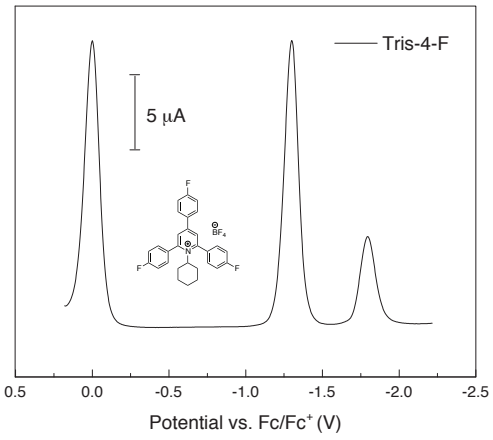



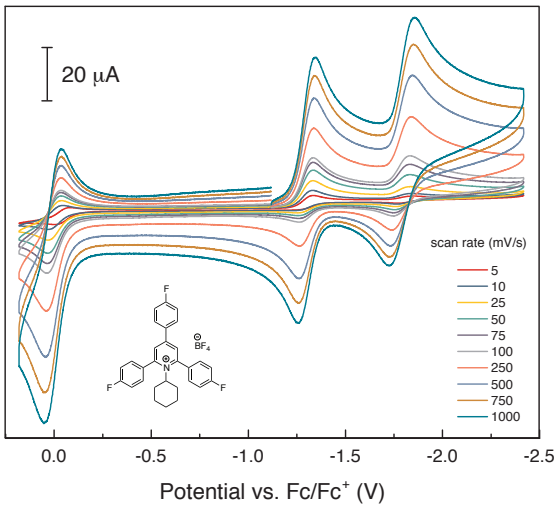
## 1c-Cy


Model
5 μA
0.5
0.0
-0.5
-1.0
-1.5
-2.0
Ptential vs. Fc/Fc+ (V)

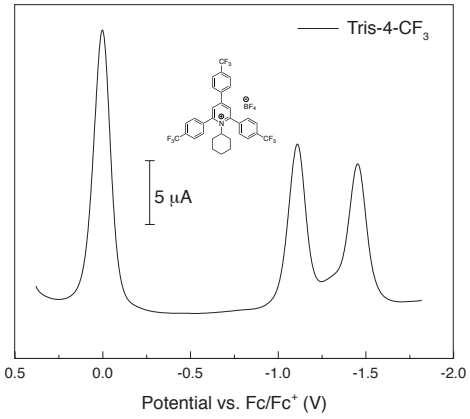

scan rate (mV/s)
5
10
25
50
75
100
250
500
750
1000
20 μA
0.0
-0.5
-1.0
-1.5
-2.0
Potential vs. Fc/Fc+ (V)

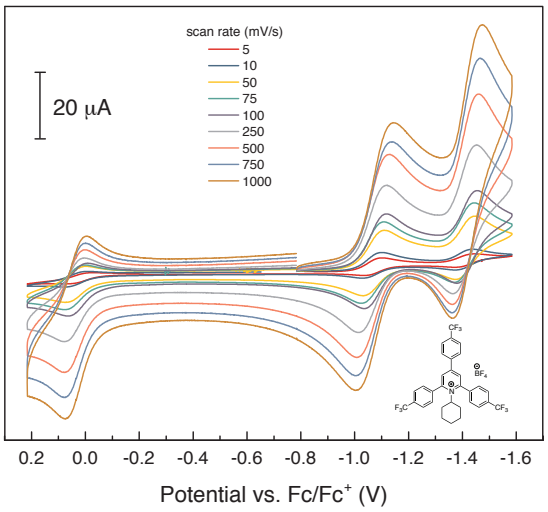
## 1d-Cy


Tris-4-F
5 μA
0.5
0.0
-0.5
-1.0
-1.5
-2.0
-2.5
Potential vs. Fc/Fc+ (V)

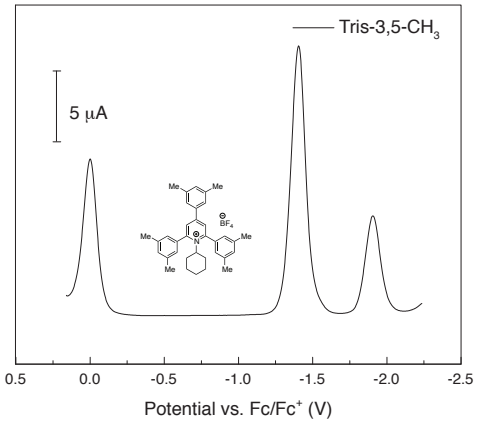

20 μA
scan rate (mV/s)
5
10
25
50
75
100
250
500
750
1000
0.0
-0.5
-1.0
-1.5
-2.0
-2.5
Potential vs. Fc/Fc+ (V)

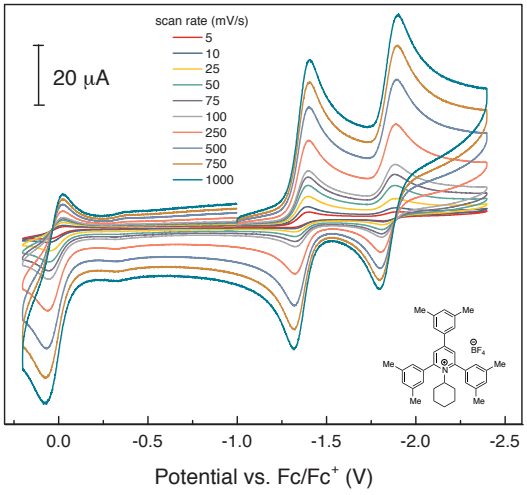
## 1e-Cy


Tris-4-CF3
5 μA
0.5
0.0
-0.5
-1.0
-1.5
-2.0
Potential vs. Fc/Fc+ (V)


scan rate (mV/s)
5
10
50
75
100
250
500
750
1000
20 μA
0.2
0.0
-0.2
-0.4
-0.6
-0.8
-1.0
-1.2
-1.4
-1.6
Potential vs. Fc/Fc+ (V)

## 1g-Cy


Tris-3,5-CH3
5 μA
0.5
0.0
-0.5
-1.0
-1.5
-2.0
-2.5
Potential vs. Fc/Fc+ (V)


scan rate (mV/s)
5
10
25
50
75
100
250
500
750
1000
20 μA
0.0
-0.5
-1.0
-1.5
-2.0
-2.5
Potential vs. Fc/Fc+ (V)

## Crystal Structures of 1c-Cy and 1c-iPr

X-ray structural analysis for **1c-Cy·0.5$CH_2Cl_2$** and **1c-i-Pr**: X-ray quality crystals of **1c-Cy·0.5$CH_2Cl_2$** and **1c-i-Pr** were obtained from slow evaporation from $CH_2Cl_2$/hexanes. Suitable crystals were selected under polarized light, mounted using viscous oil onto a plastic mesh and cooled to the data collection temperature. Data were collected on a Bruker-AXS APEX II DUO CCD diffractometer with graphite-monochromated Mo-Kα radiation (λ = 0.71073 Å). Unit cell parameters were obtained from 48 data frames, 0.5º ω, from three different sections of the Ewald sphere. The unit-cell dimensions, equivalent reflections and systematic absences in the diffraction data are consistent, uniquely, with $P2_1/n$ for **1c-Cy·0.5$CH_2Cl_2$**, and with *Cc* and *C*2/*c* for **1c-i-Pr**. Refinement in the centrosymmetric space group option for **1c-i-Pr**, *C*2/*c*, yielded chemically reasonable and computationally stable results of refinement. The data were treated with multi-scan absorption corrections.[8] Structures were solved using intrinsic phasing methods[9] and refined with full-matrix, least-squares procedures on $F^2$.[10]

Three-dimensional rigid bond restraints on anisotropic displacement parameters and geometrical restraints were applied to a dichloromethane solvent, located at an inversion center, in **1c-Cy·0.5$CH_2Cl_2$**. A disordered $BF_4^-$ anion, treated with geometrical restraints, was located in **1c-Cy·0.5$CH_2Cl_2$** with chemically equivalent atoms in the disordered contributions restrained to equal anisotropic displacement parameters with a refined site occupancy ratio of 53/47.

Three-dimensional rigid bond restraints on anisotropic displacement parameters and geometrical restraints were applied to the $BF_4^-$ in **1c-i-Pr**. Two fluorine atoms in the $BF_4^-$ counterion of **1c-i-Pr** were found disordered in two positions with a refined site occupancy of 62/38. The two methyl groups of the isopropyl moiety were found disordered over six positions, restrained to equal atomic displacement parameters, with the total occupancy restrained to two, constrained with equal $C_{Me}$-$C_{iPr}$, with refined occupancies of 55/54/48/17/14/12. Since the methyl positions cannot be assigned pairwise, the disordered positions of the isopropyl proton cannot be calculated and were ignored.

Non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms, excepting the isopropyl proton in **1c-i-Pr**, were treated as idealized contributions with geometrically calculated positions and with $U_{iso}$ equal to 1.2 $U_{eq}$ of the attached atom. Atomic scattering factors are contained in the SHELXTL program library.[10] The CIF has been deposited at the Cambridge Structural Database under CCDC 2044313 and 2044314.

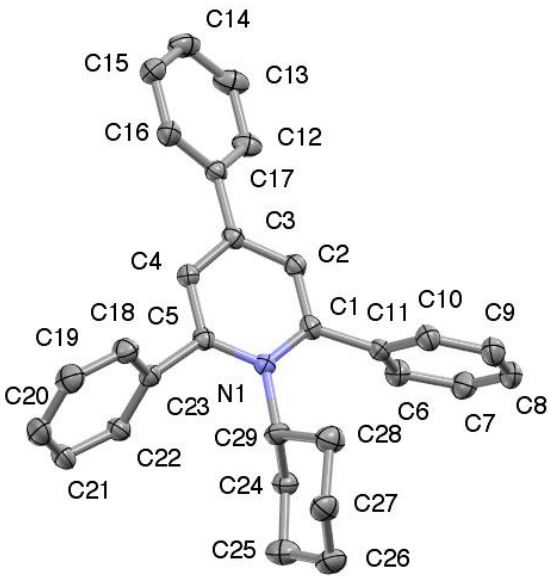



**Figure S1.** Molecular diagram of the cation in **1c-Cy·0.5CH$_2$Cl$_2$**. H-atoms and solvent atoms omitted for clarity. Ellipsoids are depicted at 50% probability.

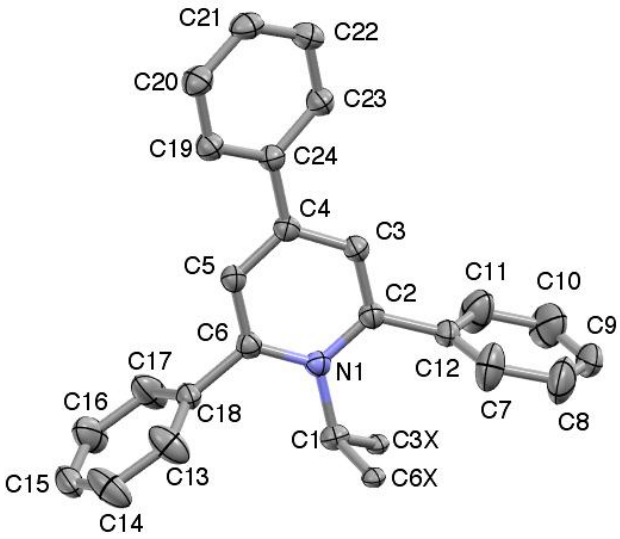



**Figure S2.** Molecular diagram of the cation in **1c-i-Pr**. H-atoms and minor disordered components omitted for clarity. Ellipsoids are depicted at 50% probability.

**Table S1.** Crystal data and structure refinement details.

| Compound | **1c-Cy·0.5CH$_2$Cl$_2$** | **1c-i-Pr** |
|---|---|---|
| Sum Formula | $C_{29.5}H_{28}BClF_4N$ | $C_{26}H_{24}BF_4N$ |
| Moiety Formula | $C_{29}H_{28}N$, $BF_4$, 0.5($CH_2Cl_2$) | $C_{26}H_{24}N$, $BF_4$ |
| Formula Weight, g/mol | 519.80 | 437.27 |
| Temperature, K | 150(2) | 200(2) |
| Crystal system | monoclinic | monoclinic |
| Space group | $P2_1/n$ | $C2/c$ |
| Cell dimensions | | |
| *a*, Å | 12.0877(17) | 16.0554(9) |
| *b*, Å | 16.723(2) | 18.7683(11) |
| *c*, Å | 12.6075(17) | 15.4095(9) |
| α, ° | 90 | 90 |
| β, ° | 92.228(2) | 105.7110(8) |
| γ, ° | 90 | 90 |
| Volume, Å$^3$ | 2546.6(6) | 4469.9(4) |
| *Z* | 4 | 8 |
| $\rho_{calc}$, g/cm$^3$ | 1.356 | 1.300 |
| μ/mm$^{-1}$ | 0.199 | 0.098 |
| F(000) | 1084 | 1824 |
| Reflections collected | 28645 | 25265 |
| Independent reflections | 5857 | 5107 |
| Data/restraints/parameters | 5857 / 116 / 359 | 5107 / 67 / 326 |
| Goodness-of-fit | 1.020 | 1.074 |
| R [I>=2σ (I)] R1/wR2 | 0.0790/0.2108 | 0.0860/0.2482 |
| R indexes [all data] R1/wR2 | 0.1147/0.2421 | 0.0931/0.2569 |
| CCDC | 2044313 | 2044314 |

## Computational Details

Optimizations of intermediates and transition states were performed using Gaussian 09[11] software with spin-unrestricted DFT using the B3LYP functional[12] and a 6-31G(d) basis set in the gas phase. For all species, vibrational frequencies were also computed at the specified level of theory to obtain thermal Gibbs Free Energy corrections (at 298 K) and to characterize the stationary points as transition states (one and only one imaginary frequency) or minima (zero imaginary frequencies). Single point energy calculations were performed on optimized geometries in solvent using the SMD-solvation model,[13] M06 functional[14] and 6-311+G(d,p) basis set. This combination has proven highly effective for all organic systems and in the cases here provided good agreement with crystallographic structural date and experimental rate data.[15]

Single-reference approaches (HF, CC) may fail to accurately capture electronic structure and hence the energy of species in the bond breaking transition state for radicals. Failure to accurately describe homolytic bond cleavage can be traced to a degeneracy or near-degeneracy of multiple electronic configurations around the corresponding transition state ('non-dynamical' electron correlation).[15] Adequate description of non-dynamical electron correlation requires multi-reference approaches (CASSCF, MRCI, etc). We assessed our system using the T1 diagnostic method developed by Lee and Taylor,[16] which estimates the importance of an admixture of additional electron configurations to a ground state description. For a typical radical dissociation transition state (N-*i*-Pr pyridinium **1k**), a T1 value of 0.037 was obtained ( CCSD/def2TZVP level), which is below the 0.044 threshold typically used as an indicator of suitability of single-reference description of electronic structure.[17] Thus, non-dynamic correlation effects are likely not critical for accurate description of these systems. Low spin contamination value (<S**2>= 0.7776 @ M06/6-311+G(d,p)) also indicates that DFT-based analysis of the system is adequate.[16]

For 'test' systems, calculations were performed in 1,4-dioxane solvent (solvent used in Ni-catalyzed C-N activation reactions). 'Realistic' systems were modeled in *N,N*-dimethyl formamide to enable comparison with experimental electrochemical data, obtained in this solvent. Single-point energies were converted to the enthalpies and Gibbs free energies using corrections from gas-phase frequency analysis. The Berne optimization procedure on preliminary structures obtained via relaxed PES scans yielded desired transition states in all the cases considered. Conformational analysis of the transition states was performed manually.

Absolute rate constants were determined from the computed activation free energies ($\Delta G^{\ddagger}$) using Eyring equation:

$$k = \frac{k_b T}{h} \exp\left(-\frac{\Delta G^{\ddagger}}{RT}\right)$$

, where $k_b = 1.38 \cdot 10^{-23} {}^{J}/_{K}$ is the Boltzmann constant, $h = 6.63 \cdot 10^{-34}\ J \cdot sec$ is the Planck constant, $R = 1.99 \cdot 10^{-3}\ {}^{kcal}/_{(mol \cdot K)}$ is a gas constant and $T$ is the absolute temperature ($T = 298.15\ K$ in our calculations).

Relative values of the reduction free energies ($\Delta G^{0}_{red},\ J/mol$) were converted to the relative reduction potentials ($E^{0}, V$) using the following equation:

$$\Delta G^{0}_{red} = -nFE^{0}$$

Where $n$ is the number of electrons transferred ($n = 1$ in our case) and $F = 96{,}485\ {}^{C}/_{mol}$ is the Faraday's constant.

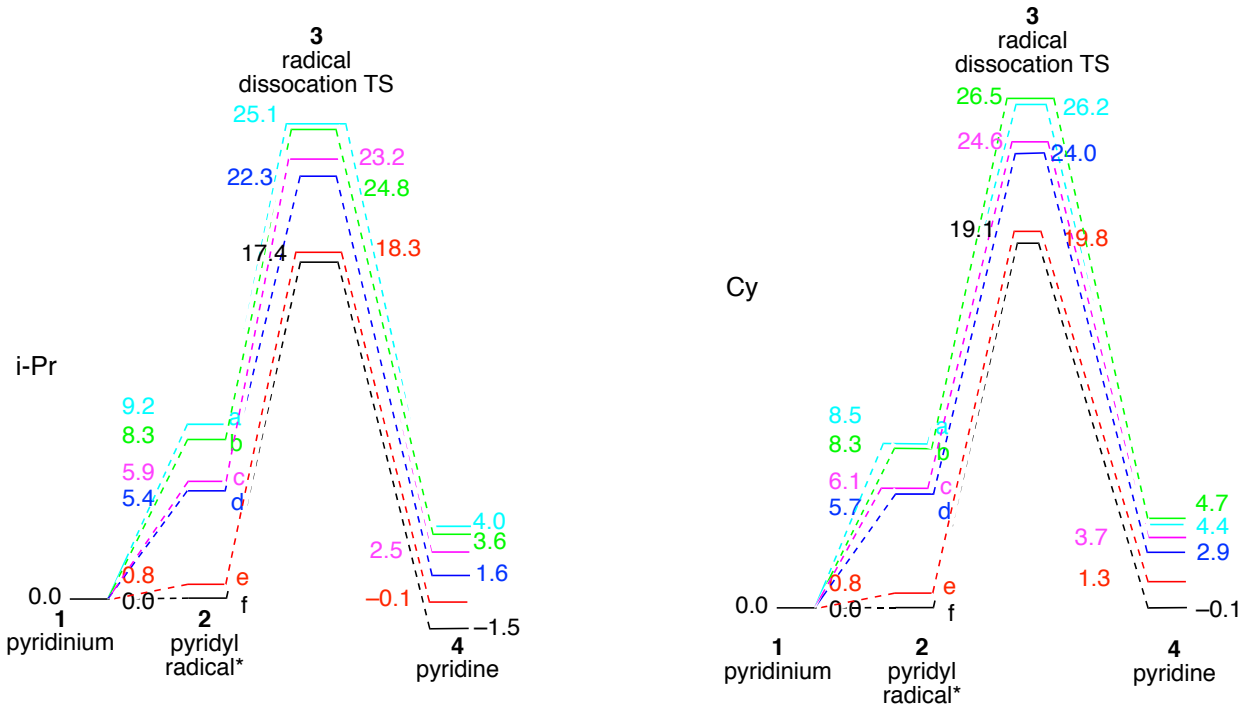


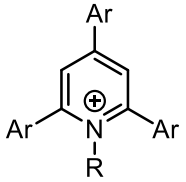

**Figure S3.** Reaction energy profile. *The values for the **2** (pyridyl radical) are relative values based on a 0.0 kcal/mol energy difference from **1**. A strong reductant would lower all values of **2**, **3** and **4**.

**Table S2.** Pyramidalization values (sum of three bond angles for nitrogen in degrees) and differences for **1-4**.

| | **1-iPr** (pyridinium) | **2**-iPr (radical) | **1**-iPr – 2-iPr | **3**-iPr (radical TS) | **2**-iPr – **3**-iPr |
|---|---|---|---|---|---|
| **a** | 359.0 | 346.9 | 12.1 | 332.5 | 14.4 |
| **b** | 359.1 | 347.8 | 11.3 | 332.5 | 15.3 |
| **c** | 359.2 | 347.9 | 11.3 | 332.5 | 15.4 |
| **d** | 359.3 | 347.6 | 11.7 | 332.4 | 15.2 |
| **e** | 359.4 | 348.7 | 10.7 | 332.2 | 16.5 |
| **f** | 359.5 | 348.0 | 11.5 | 331.8 | 16.2 |
| | | | | | |
| **h** | 356.7 | 344.1 | 12.6 | 332.0 | 12.1 |
| **i** | 359.3 | 354.8 | 4.5 | 337.9 | 16.9 |
| **j** | 359.3 | 347.8 | 11.5 | 333.4 | 14.4 |
| **k** | 360.0 | 356.5 | 3.5 | 337.3 | 19.2 |
| **l** | 360.0 | 354.9 | 5.1 | 337.0 | 17.9 |
| **m** | 359.8 | 354.7 | 5.1 | 336.2 | 18.5 |

# Coordinates and Thermochemical Data

Pyridinium salts




**Ar=Ph, R=Cy**

Zero-point correction= 0.497247 (Hartree/Particle)
Thermal correction to Energy= 0.521704
Thermal correction to Enthalpy= 0.522648
Thermal correction to Gibbs Free Energy= 0.441410
Sum of electronic and zero-point Energies= -1176.025140
Sum of electronic and thermal Energies= -1176.000683
Sum of electronic and thermal Enthalpies= -1175.999739
Sum of electronic and thermal Free Energies= -1176.080977
Single-point electronic energy (M06) = -1175.94718622

| | | | |
|---|---|---|---|
| C | 0.23381300 | 1.25696200 | -0.07663300 |
| C | 0.10608300 | -1.11939700 | -0.09906100 |
| C | 1.61866700 | 1.18536700 | -0.04879500 |
| C | 1.49156700 | -1.18402900 | -0.06648100 |
| C | 2.30212500 | -0.03850100 | -0.01028900 |
| H | 2.16122100 | 2.12265700 | -0.04558300 |
| H | 1.93872300 | -2.16780300 | -0.13754900 |
| N | -0.52830100 | 0.10427000 | -0.04841700 |
| C | -0.39422300 | 2.60681800 | -0.14116700 |
| C | -0.17658300 | 3.52044500 | 0.90187900 |
| C | -1.11084600 | 3.01532400 | -1.27892700 |
| C | -0.69188500 | 4.81402000 | 0.81934600 |
| H | 0.38358800 | 3.21321200 | 1.78069500 |
| C | -1.61465600 | 4.31210800 | -1.35903700 |
| H | -1.25303600 | 2.32744100 | -2.10744800 |
| C | -1.41071700 | 5.21121100 | -0.30923400 |
| H | -0.52794200 | 5.51057900 | 1.63595600 |
| H | -2.15871400 | 4.62305200 | -2.24580100 |
| C | -0.62185300 | -2.41582000 | -0.24790700 |
| C | -1.13379800 | -2.79685900 | -1.49768000 |
| C | -0.63469200 | -3.33716700 | 0.81037200 |
| C | -1.68769000 | -4.06554700 | -1.67108700 |
| H | -1.08063400 | -2.11088600 | -2.33807500 |
| C | -1.19868100 | -4.60062300 | 0.63470300 |
| H | -0.21309900 | -3.06010400 | 1.77274500 |
| C | -1.72817600 | -4.96554800 | -0.60468600 |
| H | -2.07726300 | -4.35242100 | -2.64321900 |
| H | -1.21625400 | -5.30125000 | 1.46405700 |
| C | 3.77019800 | -0.12046400 | 0.04787300 |
| C | 4.39856300 | -1.21869800 | 0.66568800 |
| C | 4.57260800 | 0.89485800 | -0.50663200 |
| C | 5.78639400 | -1.29337600 | 0.73385400 |
| H | 3.80057300 | -1.99895300 | 1.12729300 |
| C | 5.96042800 | 0.81007100 | -0.44810300 |
| H | 4.11386700 | 1.73445900 | -1.02007400 |
| C | 6.57075200 | -0.28134800 | 0.17486400 |
| H | 6.25664100 | -2.13870500 | 1.22684100 |
| H | 6.56662100 | 1.59275500 | -0.89382700 |
| C | -2.01756100 | 0.25025000 | 0.25177400 |
| C | -2.96526900 | -0.10820300 | -0.90205900 |
| C | -2.42178000 | -0.42758700 | 1.57181400 |
| H | -2.12042200 | 1.32144300 | 0.41632700 |
| C | -4.39276900 | 0.33438500 | -0.52558900 |
| H | -2.95983700 | -1.18538100 | -1.08395300 |
| H | -2.64381400 | 0.38472100 | -1.82716500 |
| C | -3.85477500 | 0.00894000 | 1.93514400 |
| H | -2.38903900 | -1.51620200 | 1.47744200 |
| H | -1.72313300 | -0.14103500 | 2.36769500 |
| C | -4.84573700 | -0.29387300 | 0.80120900 |
| H | -5.07840600 | 0.05847600 | -1.33443400 |
| H | -4.42652900 | 1.43030400 | -0.44650100 |
| H | -4.15950800 | -0.49865500 | 2.85709000 |
| H | -3.86309800 | 1.08606100 | 2.15428600 |
| H | -5.84356800 | 0.07172300 | 1.06820800 |
| H | -4.93413700 | -1.38232000 | 0.67630100 |
| H | 7.65378800 | -0.34350400 | 0.22367900 |
| H | -2.15973000 | -5.95240500 | -0.74244400 |
| H | -1.80579100 | 6.22052900 | -0.37454000 |

**Ar=4-Me-Ph, R=Cy**

Zero-point correction= 0.579646 (Hartree/Particle)
Thermal correction to Energy= 0.609853
Thermal correction to Enthalpy= 0.610797
Thermal correction to Gibbs Free Energy= 0.514551
Sum of electronic and zero-point Energies= -1293.902708
Sum of electronic and thermal Energies= -1293.872502
Sum of electronic and thermal Enthalpies= -1293.871558
Sum of electronic and thermal Free Energies= -1293.967803
Single-point electronic energy (M06) = -1293.83466503

| | | | |
|---|---|---|---|
| C | 0.07204500 | 1.26381400 | -0.05898200 |
| C | -0.00372000 | -1.11678600 | -0.05354400 |
| C | 1.45818600 | 1.22117700 | -0.04844400 |
| C | 1.38252000 | -1.15034100 | -0.03822100 |
| C | 2.17036500 | 0.01316200 | -0.00447900 |
| H | 1.97912500 | 2.17029900 | -0.06680200 |
| H | 1.84894500 | -2.12503000 | -0.10866200 |
| N | -0.66465700 | 0.09417100 | -0.00581700 |
| C | -0.58522100 | 2.59683000 | -0.13246700 |
| C | -0.34710500 | 3.54649200 | 0.87215600 |
| C | -1.36208500 | 2.96811500 | -1.24340000 |
| C | -0.89597700 | 4.82396600 | 0.77882300 |
| H | 0.25247400 | 3.27858700 | 1.73790500 |
| C | -1.89556000 | 4.24998600 | -1.33039800 |
| H | -1.53166200 | 2.26016000 | -2.04966600 |
| C | -1.67616500 | 5.20164200 | -0.32201500 |
| H | -0.71265400 | 5.53948200 | 1.57589900 |
| H | -2.48722200 | 4.52026900 | -2.20120700 |
| C | -0.70637700 | -2.42730600 | -0.18176400 |
| C | -1.24904200 | -2.82736300 | -1.41173400 |
| C | -0.67196100 | -3.35251900 | 0.87241600 |
| C | -1.78046600 | -4.10664200 | -1.56437100 |
| H | -1.24088800 | -2.14541100 | -2.25719700 |
| C | -1.21584900 | -4.62479100 | 0.71253400 |
| H | -0.23284700 | -3.06989800 | 1.82550200 |
| C | -1.77916000 | -5.02697900 | -0.50718400 |
| H | -2.19517700 | -4.39698600 | -2.52612800 |
| H | -1.19622900 | -5.31948100 | 1.54822400 |
| C | 3.63780400 | -0.03690500 | 0.03047000 |
| C | 4.30700600 | -1.13069500 | 0.61193400 |
| C | 4.41633000 | 1.00554400 | -0.50840400 |
| C | 5.69514200 | -1.17277600 | 0.65740800 |
| H | 3.73980300 | -1.93627000 | 1.06903900 |
| C | 5.80373800 | 0.94861400 | -0.47052100 |
| H | 3.93817200 | 1.85097000 | -0.99387400 |
| C | 6.47232400 | -0.13950000 | 0.11207500 |
| H | 6.18700700 | -2.01912200 | 1.12919300 |
| H | 6.38154800 | 1.75997300 | -0.90512500 |
| C | -2.14725600 | 0.20930600 | 0.33111400 |
| C | -3.11893500 | -0.18419800 | -0.79111300 |
| C | -2.50093400 | -0.46249700 | 1.66888100 |
| H | -2.27086000 | 1.27963600 | 0.48701700 |
| C | -4.54440100 | 0.23321400 | -0.38171700 |
| H | -3.09544400 | -1.26332900 | -0.95902000 |
| H | -2.83351000 | 0.30207400 | -1.73141200 |

| | | | |
|---|---|---|---|
| C | -3.93265900 | -0.05341600 | 2.06676200 |
| H | -2.44550200 | -1.55122400 | 1.58534300 |
| H | -1.78759400 | -0.15147400 | 2.44221700 |
| C | -4.94794100 | -0.38911900 | 0.96382400 |
| H | -5.24613100 | -0.06604600 | -1.16827700 |
| H | -4.59907600 | 1.32906100 | -0.31333200 |
| H | -4.20165300 | -0.55719000 | 3.00194500 |
| H | -3.95859400 | 1.02565900 | 2.27488000 |
| H | -5.94567000 | -0.04153600 | 1.25466900 |
| H | -5.01655900 | -1.48053400 | 0.85277800 |
| C | -2.33248500 | -6.41937800 | -0.68583700 |
| H | -1.53970600 | -7.11875300 | -0.98139200 |
| H | -2.77047300 | -6.79890100 | 0.24263900 |
| H | -3.10073400 | -6.44961700 | -1.46436600 |
| C | 7.97797300 | -0.20628600 | 0.12737700 |
| H | 8.34485600 | -0.82261200 | 0.95353400 |
| H | 8.35520000 | -0.64891200 | -0.80400800 |
| H | 8.42315500 | 0.78963900 | 0.21638600 |
| C | -2.24023400 | 6.59601700 | -0.43807400 |
| H | -2.32143700 | 7.07922000 | 0.53995900 |
| H | -1.59505700 | 7.22626600 | -1.06374200 |
| H | -3.23240900 | 6.58954900 | -0.90082100 |

**Ar=4-MeO-Ph, R=Cy**

Zero-point correction= 0.595604 (Hartree/Particle)
Thermal correction to Energy= 0.627912
Thermal correction to Enthalpy= 0.628856
Thermal correction to Gibbs Free Energy= 0.529791
Sum of electronic and zero-point Energies= -1519.506105
Sum of electronic and thermal Energies= -1519.473797
Sum of electronic and thermal Enthalpies= -1519.472853
Sum of electronic and thermal Free Energies= -1519.571917
Single-point electronic energy (M06) = -1519.43710189

| | | | |
|---|---|---|---|
| C | 0.12371600 | 1.22494700 | 0.03271100 |
| C | -0.21589900 | -1.13552400 | 0.05840800 |
| C | 1.49541900 | 1.02586500 | 0.02088200 |
| C | 1.15731700 | -1.32234300 | 0.05566100 |
| C | 2.07362900 | -0.25363900 | 0.06995700 |
| H | 2.11631200 | 1.91170500 | -0.02166700 |
| H | 1.50803600 | -2.34352300 | -0.02401500 |
| N | -0.73905200 | 0.14324100 | 0.11479200 |
| C | -0.38094300 | 2.61961800 | -0.03996800 |
| C | 0.03586200 | 3.56377100 | 0.91926400 |
| C | -1.17784500 | 3.06198000 | -1.10682200 |
| C | -0.35326800 | 4.89004500 | 0.82816000 |
| H | 0.65543500 | 3.24596700 | 1.75322800 |
| C | -1.56654000 | 4.39528200 | -1.21461200 |
| H | -1.47924100 | 2.36475100 | -1.88308600 |
| C | -1.15923500 | 5.32128500 | -0.24077300 |
| H | -0.04728200 | 5.61803200 | 1.57212500 |
| H | -2.17024600 | 4.70445900 | -2.05940400 |
| C | -1.06495100 | -2.35335300 | -0.05553300 |
| C | -1.73777500 | -2.65548200 | -1.24637000 |
| C | -1.04831800 | -3.32238600 | 0.96633300 |
| C | -2.41408400 | -3.86458700 | -1.40966800 |
| H | -1.71538800 | -1.95276500 | -2.07423000 |
| C | -1.72638700 | -4.52181100 | 0.82153100 |
| H | -0.51036300 | -3.12233900 | 1.88902100 |
| C | -2.42034500 | -4.80511000 | -0.36891600 |
| H | -2.91518200 | -4.06821300 | -2.34839600 |
| H | -1.73074700 | -5.26435800 | 1.61257600 |
| C | 3.52167100 | -0.46625200 | 0.08153400 |
| C | 4.07886500 | -1.65538500 | 0.60639300 |
| C | 4.40966100 | 0.50021100 | -0.42726300 |
| C | 5.44452800 | -1.86006300 | 0.62743900 |
| H | 3.43370300 | -2.41422500 | 1.03821700 |
| C | 5.78489300 | 0.30272100 | -0.42525900 |
| H | 4.02541100 | 1.41231200 | -0.87331600 |
| C | 6.31689600 | -0.88379600 | 0.10740300 |
| H | 5.87271700 | -2.76457400 | 1.04623400 |
| H | 6.43176900 | 1.06395300 | -0.84425000 |
| C | -2.17914300 | 0.42018800 | 0.52757400 |
| C | -3.24759800 | 0.16969500 | -0.54707500 |
| C | -2.54670300 | -0.23776100 | 1.86920900 |
| H | -2.16736800 | 1.49406300 | 0.70837100 |
| C | -4.59114300 | 0.74350100 | -0.05883300 |
| H | -3.36311300 | -0.90104600 | -0.73022500 |
| H | -2.95434700 | 0.63569600 | -1.49492100 |
| C | -3.89824000 | 0.32717200 | 2.34814300 |
| H | -2.62466900 | -1.32322500 | 1.76247700 |
| H | -1.76486100 | -0.03280000 | 2.61098800 |
| C | -4.99940400 | 0.14000000 | 1.29372800 |
| H | -5.36157100 | 0.54846900 | -0.81347900 |
| H | -4.51171100 | 1.83627000 | 0.03254800 |
| H | -4.17889500 | -0.16339600 | 3.28692500 |
| H | -3.78562000 | 1.39664400 | 2.57606200 |
| H | -5.93393800 | 0.59406500 | 1.64228700 |
| H | -5.20090000 | -0.93303700 | 1.16547200 |
| O | -3.04418500 | -6.00190200 | -0.41177000 |
| O | 7.62819600 | -1.18125600 | 0.16597200 |
| O | -1.47866500 | 6.63234600 | -0.24084900 |
| C | 8.58055300 | -0.24104600 | -0.33414500 |
| H | 8.43136800 | -0.06001600 | -1.40491900 |
| H | 8.52580800 | 0.70598200 | 0.21506900 |
| H | 9.55612000 | -0.70002300 | -0.17420400 |
| C | -3.75729200 | -6.36932600 | -1.59152200 |
| H | -3.08858500 | -6.42371800 | -2.45892800 |
| H | -4.17057300 | -7.35755400 | -1.38898300 |
| H | -4.57376700 | -5.66658500 | -1.79677300 |
| C | -2.28797500 | 7.15052900 | -1.29576700 |
| H | -1.79837100 | 7.02676100 | -2.26904100 |
| H | -3.27341400 | 6.66975000 | -1.31246200 |
| H | -2.40547200 | 8.21267100 | -1.08049900 |

**Ar=4-CF3-Ph, R=Cy**

Zero-point correction= 0.510938 (Hartree/Particle)
Thermal correction to Energy= 0.546511
Thermal correction to Enthalpy= 0.547456
Thermal correction to Gibbs Free Energy= 0.436349
Sum of electronic and zero-point Energies= -2187.104546
Sum of electronic and thermal Energies= -2187.068972
Sum of electronic and thermal Enthalpies= -2187.068028
Sum of electronic and thermal Free Energies= -2187.179135
Single-point electronic energy (M06) = -2187.04602421

| | | | |
|---|---|---|---|
| C | 0.32693700 | -1.23181400 | 0.04623000 |
| C | 0.14964500 | 1.13857000 | 0.05805100 |
| C | -1.05549700 | -1.34056700 | 0.02643700 |
| C | -1.23403100 | 1.02634800 | 0.04071800 |
| C | -1.89011000 | -0.21438000 | 0.05000800 |
| H | -1.47380200 | -2.33938100 | 0.00319400 |
| H | -1.80182200 | 1.94609700 | -0.02941300 |
| N | 0.93372000 | 0.00681000 | 0.11107600 |
| C | 1.12638200 | -2.49002800 | -0.01631400 |
| C | 1.05051200 | -3.41470700 | 1.03523800 |
| C | 1.87312700 | -2.80744700 | -1.16335600 |
| C | 1.73079600 | -4.62873900 | 0.95273500 |
| H | 0.47165900 | -3.18098700 | 1.92407100 |
| C | 2.54508200 | -4.02302900 | -1.24591300 |
| H | 1.91441000 | -2.11351800 | -1.99748400 |
| C | 2.47701200 | -4.93269800 | -0.18648400 |
| H | 1.68385200 | -5.33509200 | 1.77422100 |
| H | 3.12121800 | -4.26630100 | -2.13244700 |
| C | 0.70815100 | 2.52218700 | -0.03907200 |
| C | 1.19149600 | 3.00225200 | -1.26526100 |
| C | 0.57732100 | 3.40686500 | 1.04165100 |
| C | 1.58159300 | 4.33370200 | -1.39337000 |
| H | 1.24265700 | 2.34379100 | -2.12692400 |
| C | 0.97672500 | 4.73554700 | 0.91543700 |
| H | 0.17180100 | 3.05462700 | 1.98571200 |
| C | 1.48443300 | 5.19761500 | -0.30064800 |
| H | 1.94484100 | 4.70392400 | -2.34601200 |
| H | 0.88133500 | 5.41436900 | 1.75594100 |

| | | | |
|---|---|---|---|
| C | -3.35916900 | -0.32413900 | 0.04829500 |
| C | -4.14941600 | 0.65971600 | 0.67054500 |
| C | -3.99835000 | -1.41553200 | -0.56865200 |
| C | -5.53566700 | 0.55316400 | 0.68058900 |
| H | -3.68104100 | 1.49351200 | 1.18434100 |
| C | -5.38484300 | -1.51580600 | -0.56946400 |
| H | -3.41564400 | -2.17397400 | -1.08214300 |
| C | -6.15544100 | -0.53247500 | 0.05659400 |
| H | -6.13622900 | 1.30427400 | 1.18180500 |
| H | -5.86959200 | -2.35662100 | -1.05352300 |
| C | 1.96885800 | 6.62452400 | -0.42542400 |
| C | 3.17220400 | -6.27001100 | -0.31012300 |
| F | 3.28253200 | 6.70897100 | -0.12926700 |
| F | 1.30908900 | 7.44344800 | 0.41528200 |
| F | 1.80521700 | 7.08954100 | -1.67860700 |
| F | 3.42507800 | -6.80847400 | 0.89740900 |
| F | 4.34226000 | -6.14819400 | -0.96790200 |
| F | 2.41054000 | -7.14407000 | -0.99775900 |
| C | -7.66462700 | -0.61805100 | 0.01071200 |
| F | -8.08108000 | -1.89873900 | -0.00757900 |
| F | -8.14269300 | -0.01862300 | -1.09840400 |
| F | -8.22338900 | -0.01095100 | 1.07505300 |
| C | 2.42909100 | 0.04619200 | 0.42686300 |
| C | 3.33076700 | 0.51962200 | -0.72276500 |
| C | 2.73878500 | 0.76351400 | 1.75112600 |
| H | 2.66070700 | -1.00481400 | 0.59054400 |
| C | 4.80036100 | 0.25633100 | -0.33949200 |
| H | 3.19466500 | 1.58828200 | -0.90510500 |
| H | 3.07674300 | -0.00833100 | -1.64961200 |
| C | 4.21305000 | 0.50272100 | 2.11989800 |
| H | 2.57734200 | 1.84062500 | 1.66020100 |
| H | 2.07562700 | 0.39224400 | 2.54228200 |
| C | 5.16469700 | 0.93007800 | 0.99220600 |
| H | 5.44952900 | 0.61937100 | -1.14372900 |
| H | 4.97011500 | -0.82716500 | -0.26553800 |
| H | 4.44848100 | 1.03972500 | 3.04528000 |
| H | 4.35187400 | -0.56609500 | 2.33543900 |
| H | 6.19822200 | 0.68878500 | 1.26372600 |
| H | 5.11977900 | 2.02164800 | 0.87164100 |

**Ar=4-F-Ph, R=Cy**

Zero-point correction= 0.472361 (Hartree/Particle)
Thermal correction to Energy= 0.499356
Thermal correction to Enthalpy= 0.500300
Thermal correction to Gibbs Free Energy= 0.412879
Sum of electronic and zero-point Energies= -1473.742674
Sum of electronic and thermal Energies= -1473.715679
Sum of electronic and thermal Enthalpies= -1473.714735
Sum of electronic and thermal Free Energies= -1473.802156
Single-point electronic energy (M06) = -1473.66990635

| | | | |
|---|---|---|---|
| C | 0.08700900 | 1.26008200 | -0.06206500 |
| C | -0.00962500 | -1.11854000 | -0.05833400 |
| C | 1.47288200 | 1.20564900 | -0.05180100 |
| C | 1.37635800 | -1.16488300 | -0.04297300 |
| C | 2.17468300 | -0.00847300 | -0.00801300 |
| H | 2.00178500 | 2.15046000 | -0.06952900 |
| H | 1.83371000 | -2.14376500 | -0.11594500 |
| N | -0.66056400 | 0.09761600 | -0.00964400 |
| C | -0.55774600 | 2.60011300 | -0.13261900 |
| C | -0.31047300 | 3.54165000 | 0.88038300 |
| C | -1.32124700 | 2.98135200 | -1.25070000 |
| C | -0.83544800 | 4.82883900 | 0.79809800 |
| H | 0.28298600 | 3.26161600 | 1.74590400 |
| C | -1.84241800 | 4.26759300 | -1.34758500 |
| H | -1.49083100 | 2.27765000 | -2.06002500 |
| C | -1.59459100 | 5.17158600 | -0.31680600 |
| H | -0.66378100 | 5.56303600 | 1.57769800 |
| H | -2.42358300 | 4.58158600 | -2.20784000 |
| C | -0.72465100 | -2.42283500 | -0.18699100 |
| C | -1.26440400 | -2.81649000 | -1.42226800 |
| C | -0.69763800 | -3.34534900 | 0.87148500 |
| C | -1.80736000 | -4.08859800 | -1.58733200 |
| H | -1.24375700 | -2.13489900 | -2.26718600 |
| C | -1.24681400 | -4.61639000 | 0.72216900 |
| H | -0.25637700 | -3.06409300 | 1.82341000 |
| C | -1.79692200 | -4.96708800 | -0.50764800 |
| H | -2.22270300 | -4.40934900 | -2.53655500 |
| H | -1.24680200 | -5.33444700 | 1.53503300 |
| C | 3.64163200 | -0.07085500 | 0.02838700 |
| C | 4.29775100 | -1.17149600 | 0.61659800 |
| C | 4.42629600 | 0.96506900 | -0.51821200 |
| C | 5.68397300 | -1.23653200 | 0.66793600 |
| H | 3.72117800 | -1.97017100 | 1.07278900 |
| C | 5.81344600 | 0.90698500 | -0.48517500 |
| H | 3.95343300 | 1.80883000 | -1.01053700 |
| C | 6.42332900 | -0.19432200 | 0.11212600 |
| H | 6.19848600 | -2.07035300 | 1.13281600 |
| H | 6.42653500 | 1.68976400 | -0.91816100 |
| C | -2.14470000 | 0.22527600 | 0.32360300 |
| C | -3.11602000 | -0.15696600 | -0.80284700 |
| C | -2.50924700 | -0.44456900 | 1.65940800 |
| H | -2.25836000 | 1.29639200 | 0.48117800 |
| C | -4.53896600 | 0.27433600 | -0.39767200 |
| H | -3.10406000 | -1.23629600 | -0.97123700 |
| H | -2.82264400 | 0.32633900 | -1.74238800 |
| C | -3.93808800 | -0.02021400 | 2.05277800 |
| H | -2.46690600 | -1.53375000 | 1.57436200 |
| H | -1.79507800 | -0.14303500 | 2.43571400 |
| C | -4.95307100 | -0.34443300 | 0.94624000 |
| H | -5.24037400 | -0.01789000 | -1.18691400 |
| H | -4.58329700 | 1.37060200 | -0.32950100 |
| H | -4.21486700 | -0.52210600 | 2.98651900 |
| H | -3.95288100 | 1.05872900 | 2.26229400 |
| H | -5.94760400 | 0.01414500 | 1.23384700 |
| H | -5.03403000 | -1.43488700 | 0.83461100 |
| F | -2.09772000 | 6.40739100 | -0.40497900 |
| F | -2.32078900 | -6.18857900 | -0.65985000 |
| F | 7.75697400 | -0.25330100 | 0.15217700 |

**Ar=3,5-diF-Ph, R=Cy**

Zero-point correction= 0.446999 (Hartree/Particle)
Thermal correction to Energy= 0.476740
Thermal correction to Enthalpy= 0.477684
Thermal correction to Gibbs Free Energy= 0.383182
Sum of electronic and zero-point Energies= -1771.452589
Sum of electronic and thermal Energies= -1771.422848
Sum of electronic and thermal Enthalpies= -1771.421903
Sum of electronic and thermal Free Energies= -1771.516406
Single-point electronic energy (M06) = -1771.38252944

| | | | |
|---|---|---|---|
| C | 0.00945500 | 1.25652000 | -0.00330400 |
| C | 0.08762100 | -1.11609300 | 0.04225800 |
| C | -1.37647000 | 1.21884000 | 0.02049100 |
| C | -1.29985200 | -1.15269900 | 0.06355900 |
| C | -2.08469800 | 0.00948900 | 0.02824200 |
| H | -1.89868700 | 2.16771200 | 0.01888500 |
| H | -1.76555500 | -2.12621800 | 0.15481100 |
| N | 0.74659900 | 0.09038700 | -0.03884300 |
| C | 0.66874800 | 2.59590700 | 0.01920800 |
| C | 0.50022800 | 3.45772800 | -1.07242800 |
| C | 1.35707300 | 3.02330400 | 1.16446300 |
| C | 1.04955600 | 4.73634200 | -1.00241800 |
| H | -0.03321700 | 3.15458400 | -1.96650400 |
| C | 1.87898800 | 4.31348600 | 1.18287400 |
| H | 1.47311900 | 2.39061000 | 2.03701200 |
| C | 1.74365800 | 5.19136700 | 0.11246500 |
| C | 0.78695900 | -2.43317400 | 0.16808000 |
| C | 1.28911200 | -2.83334100 | 1.41335200 |
| C | 0.76632300 | -3.33067900 | -0.90788100 |
| C | 1.80160000 | -4.12224200 | 1.54350700 |
| H | 1.27125500 | -2.18071900 | 2.27859800 |
| C | 1.29762900 | -4.60499200 | -0.72501500 |
| H | 0.36040300 | -3.05760100 | -1.87558200 |

| | | | |
|---|---|---|---|
| C | 1.82414600 | -5.02853200 | 0.49010000 |
| C | -3.55776700 | -0.04048100 | 0.03119900 |
| C | -4.22452800 | -1.13467600 | -0.54703500 |
| C | -4.30222700 | 1.00346900 | 0.60720300 |
| C | -5.61385800 | -1.15634700 | -0.54267100 |
| H | -3.69294300 | -1.94477100 | -1.03264700 |
| C | -5.68970300 | 0.92665000 | 0.59663500 |
| H | -3.83302000 | 1.84808300 | 1.09796200 |
| C | -6.37537500 | -0.14027700 | 0.02530200 |
| C | 2.24110900 | 0.20685300 | -0.34278400 |
| C | 3.17367000 | -0.14950900 | 0.82388600 |
| C | 2.63877500 | -0.49470700 | -1.65173600 |
| H | 2.36079100 | 1.27379900 | -0.52194000 |
| C | 4.61188200 | 0.25966500 | 0.44945300 |
| H | 3.14618000 | -1.22326500 | 1.02387200 |
| H | 2.85593600 | 0.36541800 | 1.73830400 |
| C | 4.08171900 | -0.08650500 | -2.01075900 |
| H | 2.58854500 | -1.58123800 | -1.54466700 |
| H | 1.94972800 | -0.20687200 | -2.45543400 |
| C | 5.06012900 | -0.39313200 | -0.86700800 |
| H | 5.28600700 | -0.01985100 | 1.26633000 |
| H | 4.66821300 | 1.35363900 | 0.35846700 |
| H | 4.38187200 | -0.61071500 | -2.92461000 |
| H | 4.10972200 | 0.98733000 | -2.24360300 |
| H | 6.06556400 | -0.04860700 | -1.13251400 |
| H | 5.12927100 | -1.48134700 | -0.72873100 |
| H | 2.22597200 | -6.02739900 | 0.61347700 |
| H | 2.15767200 | 6.19222300 | 0.14897200 |
| H | -7.45841400 | -0.17869600 | 0.02351600 |
| F | -6.39168900 | 1.91517100 | 1.16161600 |
| F | -6.24176900 | -2.19239500 | -1.10978700 |
| F | 0.89976100 | 5.55472000 | -2.04864700 |
| F | 2.53087900 | 4.72439300 | 2.27583500 |
| F | 1.29347000 | -5.45403900 | -1.75832400 |
| F | 2.28290200 | -4.50031700 | 2.73291800 |

**Ar=3,5-diMe-Ph, R=Cy**

Zero-point correction= 0.662083 (Hartree/Particle)
Thermal correction to Energy= 0.698087
Thermal correction to Enthalpy= 0.699031
Thermal correction to Gibbs Free Energy= 0.587805
Sum of electronic and zero-point Energies= -1411.775605
Sum of electronic and thermal Energies= -1411.739601
Sum of electronic and thermal Enthalpies= -1411.738656
Sum of electronic and thermal Free Energies= -1411.849883
Single-point electronic energy (M06) = -1411.71876982

| | | | |
|---|---|---|---|
| C | -0.00219100 | 1.26170900 | 0.00259300 |
| C | 0.10511100 | -1.11635000 | 0.05329000 |
| C | -1.38721100 | 1.20250300 | 0.03250100 |
| C | -1.28084600 | -1.16721200 | 0.07958800 |
| C | -2.08340000 | -0.01501800 | 0.04312300 |
| H | -1.92075100 | 2.14476600 | 0.03551500 |
| H | -1.73335300 | -2.14570300 | 0.18085900 |
| N | 0.74783400 | 0.10097700 | -0.03717700 |
| C | 0.64004600 | 2.60646700 | 0.01896000 |
| C | 0.40208400 | 3.49338400 | -1.03919300 |
| C | 1.38953100 | 3.02872900 | 1.12803900 |
| C | 0.92903700 | 4.79042500 | -1.01611000 |
| H | -0.18579400 | 3.16687200 | -1.89332700 |
| C | 1.91234400 | 4.32426100 | 1.18190000 |
| H | 1.54396900 | 2.35398900 | 1.96598200 |
| C | 1.67634700 | 5.18333300 | 0.10001100 |
| C | 0.82541300 | -2.41938300 | 0.18599700 |
| C | 1.35552100 | -2.80089600 | 1.42575300 |
| C | 0.80310900 | -3.33883000 | -0.87112400 |
| C | 1.90034200 | -4.07764300 | 1.60785400 |
| H | 1.32299300 | -2.10981900 | 2.26383100 |
| C | 1.35153200 | -4.61748900 | -0.71905600 |
| H | 0.36082600 | -3.05476800 | -1.82274600 |
| C | 1.89340700 | -4.96449600 | 0.52470000 |
| C | -3.55293900 | -0.08329100 | 0.05293500 |
| C | -4.21536000 | -1.18666400 | -0.51352000 |
| C | -4.31520200 | 0.95042800 | 0.62533900 |
| C | -5.60928600 | -1.26331800 | -0.52431400 |
| H | -3.64207400 | -1.97874900 | -0.98737800 |
| C | -5.70993800 | 0.89187300 | 0.64397900 |
| H | -3.81983600 | 1.79193700 | 1.10131300 |
| C | -6.33595600 | -0.21838300 | 0.06161200 |
| C | 2.22697100 | 0.23035200 | -0.38025100 |
| C | 3.20036900 | -0.13158200 | 0.75093700 |
| C | 2.58985900 | -0.45827800 | -1.70663000 |
| H | 2.33691800 | 1.29951200 | -0.55306100 |
| C | 4.62293900 | 0.28975700 | 0.33597000 |
| H | 3.18346000 | -1.20699100 | 0.94241800 |
| H | 2.90793500 | 0.37348800 | 1.67914700 |
| C | 4.01819800 | -0.04140500 | -2.10813600 |
| H | 2.54457600 | -1.54589300 | -1.60671500 |
| H | 1.87477400 | -0.16592900 | -2.48565900 |
| C | 5.03408300 | -0.35153200 | -0.99829200 |
| H | 5.32620000 | 0.01024900 | 1.12849300 |
| H | 4.66868900 | 1.38465800 | 0.24844800 |
| H | 4.29393000 | -0.55618000 | -3.03538500 |
| H | 4.03477600 | 1.03476800 | -2.33182300 |
| H | 6.02981900 | -0.00124100 | -1.29285200 |
| H | 5.11048900 | -1.44051200 | -0.86946800 |
| H | 2.30953300 | -5.96121400 | 0.65805700 |
| H | 2.08228900 | 6.19251700 | 0.13252500 |
| H | -7.42309600 | -0.27176000 | 0.06612000 |
| C | -6.32294400 | -2.43339400 | -1.15926900 |
| H | -5.62016800 | -3.21003100 | -1.47500000 |
| H | -7.03657700 | -2.88757700 | -0.46256800 |
| H | -6.89107100 | -2.11788300 | -2.04267300 |
| C | -6.53046900 | 1.98745300 | 1.28252000 |
| H | -5.89803400 | 2.79527000 | 1.66220400 |
| H | -7.23674800 | 2.42199900 | 0.56555400 |
| H | -7.12038600 | 1.60142000 | 2.12218300 |
| C | 2.48226800 | -4.49039800 | 2.93952000 |
| H | 2.12833300 | -5.48310600 | 3.23764000 |
| H | 3.57744500 | -4.53957100 | 2.89324000 |
| H | 2.21563400 | -3.78477100 | 3.73204800 |
| C | 1.36155200 | -5.60087300 | -1.86557800 |
| H | 2.37638800 | -5.73631400 | -2.25985800 |
| H | 1.00644000 | -6.58690300 | -1.54685900 |
| H | 0.72816600 | -5.26367800 | -2.69148300 |
| C | 2.69129300 | 4.80043100 | 2.38534700 |
| H | 3.62633300 | 5.28695500 | 2.08656200 |
| H | 2.11555900 | 5.53571600 | 2.96077900 |
| H | 2.93979400 | 3.97437700 | 3.05825000 |
| C | 0.71168100 | 5.73703700 | -2.17268100 |
| H | 0.48222500 | 6.74854300 | -1.82160200 |
| H | 1.61142500 | 5.80814200 | -2.79686000 |
| H | -0.10963700 | 5.40632200 | -2.81549600 |

**Ar=Ph, R=iPr**

Zero-point correction= 0.430433 (Hartree/Particle)
Thermal correction to Energy= 0.453250
Thermal correction to Enthalpy= 0.454194
Thermal correction to Gibbs Free Energy= 0.376625
Sum of electronic and zero-point Energies= -1059.354015
Sum of electronic and thermal Energies= -1059.331198
Sum of electronic and thermal Enthalpies= -1059.330254
Sum of electronic and thermal Free Energies= -1059.407823
Single-point electronic energy (M06) = -1059.26985393

| | | | |
|---|---|---|---|
| C | -2.50856000 | 0.36219600 | 0.50070800 |
| H | -2.55033700 | 1.43367100 | 0.67844900 |
| C | -0.23700500 | 1.27466800 | 0.03341700 |
| C | -0.46984800 | -1.09498900 | 0.01751000 |
| C | 1.14231800 | 1.14204100 | -0.02385000 |
| C | 0.91065500 | -1.22066700 | -0.03464100 |
| C | 1.77233500 | -0.11122000 | -0.02755400 |
| H | 1.72476400 | 2.05451900 | -0.05352500 |

| | | | |
|---|---|---|---|
| H | 1.30892700 | -2.22280400 | -0.13405100 |
| N | -1.04420300 | 0.15562700 | 0.10720900 |
| C | -0.81095100 | 2.64963500 | 0.00690400 |
| C | -0.50054700 | 3.54986800 | 1.03812600 |
| C | -1.57166800 | 3.09011100 | -1.08957800 |
| C | -0.96700100 | 4.86331300 | 0.98488800 |
| H | 0.09351900 | 3.21740300 | 1.88488300 |
| C | -2.02553700 | 4.40653300 | -1.14133500 |
| H | -1.78651300 | 2.41122200 | -1.90982600 |
| C | -1.72877400 | 5.29291800 | -0.10304600 |
| H | -0.73174500 | 5.55004300 | 1.79229600 |
| H | -2.60419200 | 4.74200300 | -1.99667300 |
| C | -1.26736500 | -2.35379600 | -0.08241000 |
| C | -1.90693100 | -2.69261100 | -1.28475500 |
| C | -1.23189300 | -3.28775800 | 0.96477700 |
| C | -2.53533400 | -3.93084100 | -1.41961600 |
| H | -1.89425700 | -1.99987400 | -2.12100800 |
| C | -1.87086000 | -4.51987600 | 0.82861500 |
| H | -0.71505300 | -3.04379200 | 1.88893900 |
| C | -2.52572300 | -4.84184700 | -0.36186600 |
| H | -3.02280700 | -4.18586800 | -2.35576600 |
| H | -1.85021700 | -5.22962000 | 1.65007500 |
| C | 3.23591200 | -0.25798000 | -0.05991400 |
| C | 3.85166300 | -1.38589400 | 0.51595100 |
| C | 4.04710900 | 0.72329200 | -0.66130900 |
| C | 5.23623600 | -1.52266900 | 0.49745300 |
| H | 3.24937800 | -2.14078600 | 1.01280100 |
| C | 5.43060400 | 0.57619300 | -0.68975900 |
| H | 3.59566100 | 1.58486100 | -1.14389800 |
| C | 6.02887900 | -0.54424800 | -0.10790400 |
| H | 5.69792600 | -2.39012500 | 0.95905400 |
| H | 6.04241700 | 1.33298100 | -1.17107000 |
| C | -3.51341300 | 0.05156700 | -0.61138000 |
| H | -3.68688300 | -1.01759800 | -0.73485300 |
| H | -4.46628100 | 0.51741300 | -0.33852000 |
| H | -3.20239700 | 0.47407300 | -1.57149000 |
| C | -2.83331700 | -0.32077600 | 1.83276000 |
| H | -3.79711100 | 0.06720100 | 2.17888400 |
| H | -2.92200500 | -1.40437300 | 1.74716400 |
| H | -2.08608900 | -0.08098600 | 2.59628900 |
| H | -3.01646000 | -5.80450900 | -0.46931000 |
| H | -2.08570900 | 6.31754700 | -0.14563700 |
| H | 7.10897800 | -0.65496800 | -0.12681800 |

**Ar=4-Me-Ph, R=iPr**

Zero-point correction= 0.512941 (Hartree/Particle)
Thermal correction to Energy= 0.541465
Thermal correction to Enthalpy= 0.542409
Thermal correction to Gibbs Free Energy= 0.449789
Sum of electronic and zero-point Energies= -1177.231683
Sum of electronic and thermal Energies= -1177.203159
Sum of electronic and thermal Enthalpies= -1177.202215
Sum of electronic and thermal Free Energies= -1177.294835
Single-point electronic energy (M06) = -1177.15744730

| | | | |
|---|---|---|---|
| C | -0.51421400 | -2.55185300 | 0.59380500 |
| H | -1.58749000 | -2.52951700 | 0.76470400 |
| C | -1.29856400 | -0.24865600 | 0.05257300 |
| C | 1.05658900 | -0.61365400 | 0.06682500 |
| C | -1.08596500 | 1.12026100 | -0.01549100 |
| C | 1.26002200 | 0.75661700 | 0.00798900 |
| C | 0.20045200 | 1.68059500 | -0.00323200 |
| H | -1.96360800 | 1.75222900 | -0.06803300 |
| H | 2.28391500 | 1.09608900 | -0.08675000 |
| N | -0.22629000 | -1.11657900 | 0.15136100 |
| C | -2.70093800 | -0.74312800 | 0.01287800 |
| C | -3.61629900 | -0.31802800 | 0.98723900 |
| C | -3.16271800 | -1.54818100 | -1.04335800 |
| C | -4.95198500 | -0.70975300 | 0.91821200 |
| H | -3.27874000 | 0.30480000 | 1.81117600 |
| C | -4.50028900 | -1.92338200 | -1.10717700 |
| H | -2.47958300 | -1.86104100 | -1.82780200 |
| C | -5.42032400 | -1.51465900 | -0.12835500 |
| H | -5.64170700 | -0.38263100 | 1.69152200 |
| H | -4.83980200 | -2.53901200 | -1.93618200 |
| C | 2.26529200 | -1.48288000 | -0.02213700 |
| C | 2.55801200 | -2.18203000 | -1.20293200 |
| C | 3.21876900 | -1.47028600 | 1.00712700 |
| C | 3.75633200 | -2.88131700 | -1.32859400 |
| H | 1.85855100 | -2.16372400 | -2.03357600 |
| C | 4.40857300 | -2.18284900 | 0.87574800 |
| H | 3.02099300 | -0.91558800 | 1.92052700 |
| C | 4.70097900 | -2.90071700 | -0.29256900 |
| H | 3.96468800 | -3.41413800 | -2.25275800 |
| H | 5.12448200 | -2.17642600 | 1.69342100 |
| C | 0.42885600 | 3.13066200 | -0.04304300 |
| C | 1.59227100 | 3.69126300 | 0.51890200 |
| C | -0.50749900 | 4.00075800 | -0.63324800 |
| C | 1.80152200 | 5.06424100 | 0.49730900 |
| H | 2.31969500 | 3.05449200 | 1.01386300 |
| C | -0.28261200 | 5.37165900 | -0.66333400 |
| H | -1.40119000 | 3.60421100 | -1.10574100 |
| C | 0.87335500 | 5.93233400 | -0.09913700 |
| H | 2.69754500 | 5.47348700 | 0.95626200 |
| H | -1.01442400 | 6.02063800 | -1.13675000 |
| C | -0.25128900 | -3.61662800 | -0.47410600 |
| H | 0.80714500 | -3.85669600 | -0.57696200 |
| H | -0.77536100 | -4.52928000 | -0.17066800 |
| H | -0.64367300 | -3.32023400 | -1.45135400 |
| C | 0.14413600 | -2.86138900 | 1.94197900 |
| H | -0.28704500 | -3.79540100 | 2.31746700 |
| H | 1.22368200 | -2.99859000 | 1.86719500 |
| H | -0.06771100 | -2.07840000 | 2.67743900 |
| C | 6.00665000 | -3.64095000 | -0.44634100 |
| H | 6.76124400 | -3.00398800 | -0.92579100 |
| H | 6.40894900 | -3.95074200 | 0.52283600 |
| H | 5.89080500 | -4.53259600 | -1.07033100 |
| C | -6.87241900 | -1.91272000 | -0.22058000 |
| H | -7.39044500 | -1.76761900 | 0.73163500 |
| H | -7.39418100 | -1.31173300 | -0.97628200 |
| H | -6.98141100 | -2.96263700 | -0.51249000 |
| C | 1.12366300 | 7.41764200 | -0.15249300 |
| H | 1.66901600 | 7.76433000 | 0.73087900 |
| H | 1.72926200 | 7.67718500 | -1.03088200 |
| H | 0.18828600 | 7.98074600 | -0.22285900 |

**Ar=4-MeO-Ph, R=iPr**

Zero-point correction= 0.528908 (Hartree/Particle)
Thermal correction to Energy= 0.559487
Thermal correction to Enthalpy= 0.560431
Thermal correction to Gibbs Free Energy= 0.465519
Sum of electronic and zero-point Energies= -1402.835327
Sum of electronic and thermal Energies= -1402.804748
Sum of electronic and thermal Enthalpies= -1402.803803
Sum of electronic and thermal Free Energies= -1402.898716
Single-point electronic energy (M06) = -1402.76004689

| | | | |
|---|---|---|---|
| C | 1.99019600 | 1.62347400 | 0.88698400 |
| H | 2.80433800 | 0.92539800 | 1.06673300 |
| C | 1.21222100 | -0.62803900 | 0.15169300 |
| C | -0.40695900 | 1.12488900 | 0.18302500 |
| C | 0.19501800 | -1.56152200 | 0.02091300 |
| C | -1.41501400 | 0.18281800 | 0.06210100 |
| C | -1.16323900 | -1.20242300 | 0.01520100 |
| H | 0.49316600 | -2.59790500 | -0.07390600 |
| H | -2.42146900 | 0.56104700 | -0.06516400 |
| N | 0.90935500 | 0.71580200 | 0.30237600 |
| C | 2.61511700 | -1.10853200 | 0.12132800 |
| C | 3.02656500 | -2.12787500 | 1.00359500 |
| C | 3.52772000 | -0.65847000 | -0.84569100 |
| C | 4.30587400 | -2.65371500 | 0.93675400 |
| H | 2.33926900 | -2.49408000 | 1.76112400 |
| C | 4.81275300 | -1.18806800 | -0.93018000 |
| H | 3.22536300 | 0.09570900 | -1.56636100 |

| | | | |
|---|---|---|---|
| C | 5.21454600 | -2.19001200 | -0.03192900 |
| H | 4.63203300 | -3.42726200 | 1.62397700 |
| H | 5.48480000 | -0.82720200 | -1.69952700 |
| C | -0.79841400 | 2.55853300 | 0.12088400 |
| C | -0.47675300 | 3.34818600 | -0.99089100 |
| C | -1.66222300 | 3.09735400 | 1.09456900 |
| C | -0.96167700 | 4.64930800 | -1.12014700 |
| H | 0.13945200 | 2.93877000 | -1.78584900 |
| C | -2.13954900 | 4.39312100 | 0.98498400 |
| H | -1.94582300 | 2.49605200 | 1.95414000 |
| C | -1.79193900 | 5.18569100 | -0.12433000 |
| H | -0.70115900 | 5.22627800 | -1.99935500 |
| H | -2.79017500 | 4.81869100 | 1.74177100 |
| C | -2.23871100 | -2.18900600 | -0.08973200 |
| C | -3.53466600 | -1.89891000 | 0.37760100 |
| C | -2.01693600 | -3.46705800 | -0.65346800 |
| C | -4.56502900 | -2.82754600 | 0.30145000 |
| H | -3.74057600 | -0.94198900 | 0.84751100 |
| C | -3.03472000 | -4.39557700 | -0.74847000 |
| H | -1.04348100 | -3.72364800 | -1.05939400 |
| C | -4.32350100 | -4.08890000 | -0.26919900 |
| H | -5.54296300 | -2.57059300 | 0.69023500 |
| H | -2.86949000 | -5.36886300 | -1.19823100 |
| C | 2.52323700 | 2.70026600 | -0.06167100 |
| H | 1.85680900 | 3.55994100 | -0.13595300 |
| H | 3.48184100 | 3.05104200 | 0.33578000 |
| H | 2.70620000 | 2.30789900 | -1.06627400 |
| C | 1.56705500 | 2.17680000 | 2.25205600 |
| H | 2.45116200 | 2.61750700 | 2.72480000 |
| H | 0.80558000 | 2.95495100 | 2.17796800 |
| H | 1.20160000 | 1.38002000 | 2.90806900 |
| O | 6.43245600 | -2.76904800 | -0.01672100 |
| O | -2.31215800 | 6.43098700 | -0.14008700 |
| O | -5.24325200 | -5.06172000 | -0.40434300 |
| C | -6.58005700 | -4.82671600 | 0.04209300 |
| H | -7.12749000 | -5.74258700 | -0.18022700 |
| H | -6.60795200 | -4.63541000 | 1.12103200 |
| H | -7.03388800 | -3.98732400 | -0.49724400 |
| C | 7.41053100 | -2.35568700 | -0.97077000 |
| H | 7.65092300 | -1.29205000 | -0.85591300 |
| H | 8.29689300 | -2.95397900 | -0.75963800 |
| H | 7.07266300 | -2.55137500 | -1.99533800 |
| C | -2.01514400 | 7.29212800 | -1.23854500 |
| H | -2.38419000 | 6.87290000 | -2.18219200 |
| H | -2.53537000 | 8.22659600 | -1.02773700 |
| H | -0.93773600 | 7.48203200 | -1.31350500 |

**Ar=4-CF3-Ph, R=iPr**

Zero-point correction= 0.444179 (Hartree/Particle)
Thermal correction to Energy= 0.478098
Thermal correction to Enthalpy= 0.479042
Thermal correction to Gibbs Free Energy= 0.371437
Sum of electronic and zero-point Energies= -2070.432945
Sum of electronic and thermal Energies= -2070.399026
Sum of electronic and thermal Enthalpies= -2070.398082
Sum of electronic and thermal Free Energies= -2070.505687
Single-point electronic energy (M06) = -2070.36886974

| | | | |
|---|---|---|---|
| C | 0.41846100 | -2.78173900 | -0.52544800 |
| H | 1.49480300 | -2.82543000 | -0.66887700 |
| C | 1.30295200 | -0.48535500 | -0.12051600 |
| C | -1.06206600 | -0.73617600 | -0.14524000 |
| C | 1.16048500 | 0.89358600 | -0.06820500 |
| C | -1.20070400 | 0.64389300 | -0.09856700 |
| C | -0.09767600 | 1.51205400 | -0.08045300 |
| H | 2.06744900 | 1.48446400 | -0.03010000 |
| H | -2.20790200 | 1.03585500 | -0.02679800 |
| N | 0.19278600 | -1.30172900 | -0.20214200 |
| C | 2.68574500 | -1.04464700 | -0.08011300 |
| C | 3.57237800 | -0.77260800 | -1.13262500 |
| C | 3.14418500 | -1.74926300 | 1.04540100 |
| C | 4.89127600 | -1.21836900 | -1.07141400 |
| H | 3.22878900 | -0.22398000 | -2.00476600 |
| C | 4.46437400 | -2.18554900 | 1.10742400 |
| H | 2.47616200 | -1.94109700 | 1.87976700 |
| C | 5.33727800 | -1.92272800 | 0.04816900 |
| H | 5.57033600 | -1.02180700 | -1.89394100 |
| H | 4.81705200 | -2.72896800 | 1.97742800 |
| C | -2.32232500 | -1.53880800 | -0.07582900 |
| C | -2.72944500 | -2.10394500 | 1.14201800 |
| C | -3.19424300 | -1.57024600 | -1.17404300 |
| C | -3.97059100 | -2.72831000 | 1.24577400 |
| H | -2.08839300 | -2.03772600 | 2.01573900 |
| C | -4.43111000 | -2.20368700 | -1.07178800 |
| H | -2.90441600 | -1.10540700 | -2.11195100 |
| C | -4.81759100 | -2.78621800 | 0.13687600 |
| H | -4.28716700 | -3.15365200 | 2.19209300 |
| H | -5.10000100 | -2.23165200 | -1.92502300 |
| C | -0.25669700 | 2.97579900 | -0.04170100 |
| C | -1.36182700 | 3.58942200 | -0.66096600 |
| C | 0.69035200 | 3.78592200 | 0.61077900 |
| C | -1.51202400 | 4.97073600 | -0.63258700 |
| H | -2.08847700 | 2.99035100 | -1.20124100 |
| C | 0.53204700 | 5.16698400 | 0.65208300 |
| H | 1.53653800 | 3.33800700 | 1.12240700 |
| C | -0.56787600 | 5.76110500 | 0.02914100 |
| H | -2.35423000 | 5.43760700 | -1.13183600 |
| H | 1.26095700 | 5.78368500 | 1.16603800 |
| C | 0.07756500 | -3.72835700 | 0.62808600 |
| H | -0.99488700 | -3.89235300 | 0.73611300 |
| H | 0.54338500 | -4.69575400 | 0.41330500 |
| H | 0.48056100 | -3.37187400 | 1.58099500 |
| C | -0.22032400 | -3.17497400 | -1.86084600 |
| H | 0.19381200 | -4.14581400 | -2.15219500 |
| H | -1.30395000 | -3.28112000 | -1.80271300 |
| H | 0.02949000 | -2.45869900 | -2.65034400 |
| C | -6.13856500 | -3.51529400 | 0.23979500 |
| C | 6.78467700 | -2.35126100 | 0.14468200 |
| F | -5.98063000 | -4.82873300 | -0.02331600 |
| F | -7.03767700 | -3.02939900 | -0.63650500 |
| F | -6.65895700 | -3.40953600 | 1.47746500 |
| F | 7.31621000 | -2.56054500 | -1.07452800 |
| F | 6.91035600 | -3.48723100 | 0.85776400 |
| F | 7.52348900 | -1.40347600 | 0.75539600 |
| C | -0.77286300 | 7.25719500 | 0.11331900 |
| F | 0.39246200 | 7.90482100 | 0.30027000 |
| F | -1.58456200 | 7.56881200 | 1.14387700 |
| F | -1.34230100 | 7.73445400 | -1.01024000 |

**Ar=4-F-Ph, R=iPr**

Zero-point correction= 0.405660 (Hartree/Particle)
Thermal correction to Energy= 0.430951
Thermal correction to Enthalpy= 0.431895
Thermal correction to Gibbs Free Energy= 0.348316
Sum of electronic and zero-point Energies= -1357.071317
Sum of electronic and thermal Energies= -1357.046026
Sum of electronic and thermal Enthalpies= -1357.045081
Sum of electronic and thermal Free Energies= -1357.128661
Single-point electronic energy (M06) = -1356.99265502

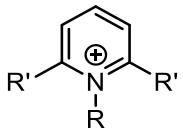
| | | | |
|---|---|---|---|
| C | -0.06431300 | -2.61396400 | 0.54188000 |
| H | -1.12567400 | -2.78228900 | 0.70452900 |
| C | -1.23455200 | -0.46722300 | 0.04997200 |
| C | 1.14689700 | -0.42141300 | 0.05436000 |
| C | -1.26170200 | 0.91824500 | -0.00880900 |
| C | 1.11125800 | 0.96378100 | -0.00015800 |
| C | -0.09122300 | 1.69232700 | -0.00341100 |
| H | -2.23589200 | 1.38920700 | -0.05051300 |
| H | 2.06152400 | 1.47387200 | -0.09742900 |
| N | -0.02903400 | -1.13925500 | 0.13589800 |
| C | -2.53323800 | -1.19396800 | 0.01513200 |
| C | -3.49008100 | -0.94992800 | 1.01477200 |
| C | -2.86660300 | -2.03647200 | -1.06097200 |
| C | -4.74410200 | -1.55271900 | 0.96070700 |

| | | | |
|---|---|---|---|
| H | -3.24738300 | -0.29712000 | 1.84823000 |
| C | -4.12006300 | -2.63577400 | -1.12995000 |
| H | -2.15298000 | -2.20743600 | -1.86133200 |
| C | -5.03959500 | -2.38739200 | -0.11316500 |
| H | -5.48876700 | -1.38422600 | 1.73100100 |
| H | -4.39717400 | -3.27885600 | -1.95820100 |
| C | 2.48983600 | -1.06694900 | -0.02951200 |
| C | 2.91676200 | -1.67524700 | -1.22118100 |
| C | 3.40734000 | -0.90689900 | 1.02214800 |
| C | 4.21859000 | -2.15412200 | -1.34733300 |
| H | 2.23824700 | -1.75736700 | -2.06463400 |
| C | 4.70822800 | -1.39115500 | 0.91221100 |
| H | 3.09876200 | -0.41235100 | 1.93876300 |
| C | 5.09289800 | -2.01124200 | -0.27349700 |
| H | 4.56531800 | -2.62012700 | -2.26331200 |
| H | 5.42298800 | -1.28868600 | 1.72149800 |
| C | -0.11696200 | 3.16001500 | -0.04197300 |
| C | 0.94331500 | 3.91037100 | 0.50657700 |
| C | -1.19964800 | 3.85195600 | -0.62264700 |
| C | 0.92481900 | 5.29867200 | 0.48642700 |
| H | 1.77578500 | 3.40736000 | 0.98846100 |
| C | -1.22501400 | 5.23984700 | -0.66128700 |
| H | -2.01455800 | 3.30424000 | -1.08527700 |
| C | -0.16102200 | 5.94455600 | -0.10159900 |
| H | 1.72676500 | 5.88561200 | 0.92054800 |
| H | -2.04410600 | 5.78190300 | -1.12102400 |
| C | 0.38281600 | -3.58588100 | -0.55297300 |
| H | 1.46744600 | -3.63909200 | -0.64990300 |
| H | 0.02171900 | -4.58347700 | -0.28142400 |
| H | -0.04802600 | -3.33254300 | -1.52630100 |
| C | 0.63170900 | -2.84348000 | 1.88725300 |
| H | 0.35288200 | -3.84225400 | 2.23905800 |
| H | 1.71964200 | -2.80800000 | 1.81738500 |
| H | 0.29632400 | -2.12161300 | 2.63902500 |
| F | 6.34270200 | -2.47286600 | -0.38870300 |
| F | -0.18220200 | 7.27937400 | -0.13014300 |
| F | -6.24357700 | -2.96513200 | -0.17429300 |

**Ar=3,5-diF-Ph, R=iPr**

Zero-point correction= 0.380299 (Hartree/Particle)
Thermal correction to Energy= 0.408346
Thermal correction to Enthalpy= 0.409290
Thermal correction to Gibbs Free Energy= 0.318636
Sum of electronic and zero-point Energies= -1654.780871
Sum of electronic and thermal Energies= -1654.752824
Sum of electronic and thermal Enthalpies= -1654.751880
Sum of electronic and thermal Free Energies= -1654.842533
Single-point electronic energy (M06) = -1654.70520829

| | | | |
|---|---|---|---|
| C | 0.45742700 | -2.62529800 | -0.55420600 |
| H | 1.52493100 | -2.62398800 | -0.75863400 |
| C | 1.29007300 | -0.31927900 | -0.10149600 |
| C | -1.06498500 | -0.63022500 | -0.06166900 |
| C | 1.11760200 | 1.05319000 | -0.00744500 |
| C | -1.23657200 | 0.74426100 | 0.02745200 |
| C | -0.15550600 | 1.63872200 | 0.03323700 |
| H | 2.01089900 | 1.66505700 | 0.01750800 |
| H | -2.25041100 | 1.10815600 | 0.13998500 |
| N | 0.20012600 | -1.16199800 | -0.17429600 |
| C | 2.68609300 | -0.84894300 | -0.11348200 |
| C | 3.51659500 | -0.56405600 | -1.20540200 |
| C | 3.18751000 | -1.53322300 | 1.00368900 |
| C | 4.84127100 | -0.99441200 | -1.16409500 |
| H | 3.15613000 | -0.03033400 | -2.07778200 |
| C | 4.52096800 | -1.93263600 | 0.99462000 |
| H | 2.57872600 | -1.73654000 | 1.87730800 |
| C | 5.37064300 | -1.68034800 | -0.07719100 |
| C | -2.30335700 | -1.46502400 | 0.02418800 |
| C | -2.62843900 | -2.10557300 | 1.22722400 |
| C | -3.21793200 | -1.44767800 | -1.03778000 |
| C | -3.85836300 | -2.75247800 | 1.32774700 |
| H | -1.96753500 | -2.09068800 | 2.08609600 |
| C | -4.42993900 | -2.11684800 | -0.88665100 |
| H | -3.00340900 | -0.94094800 | -1.97214300 |
| C | -4.77694200 | -2.77996300 | 0.28520200 |
| C | -0.34871700 | 3.09776600 | 0.10867100 |
| C | -1.50145500 | 3.68289300 | -0.44370300 |
| C | 0.61652800 | 3.91040400 | 0.72831600 |
| C | -1.65831000 | 5.06162400 | -0.37088200 |
| H | -2.25479700 | 3.10021900 | -0.96107500 |
| C | 0.40433600 | 5.28253200 | 0.78681200 |
| H | 1.50177700 | 3.50172400 | 1.20133200 |
| C | -0.72288500 | 5.88882900 | 0.24211200 |
| C | 0.21711100 | -3.61444200 | 0.58837400 |
| H | -0.84137400 | -3.81657300 | 0.75371000 |
| H | 0.70004900 | -4.55912300 | 0.31763800 |
| H | 0.66514100 | -3.27215800 | 1.52592100 |
| C | -0.24274700 | -3.00384600 | -1.86228700 |
| H | 0.18949800 | -3.94939700 | -2.20588000 |
| H | -1.31664500 | -3.15248400 | -1.74684400 |
| H | -0.06567200 | -2.25668100 | -2.64274000 |
| H | -5.72873300 | -3.28846700 | 0.38510000 |
| H | -0.86671700 | 6.96173600 | 0.29370900 |
| H | 6.40576100 | -2.00104500 | -0.06284600 |
| F | -2.74860700 | 5.61349600 | -0.91453100 |
| F | 1.31780500 | 6.04792300 | 1.39382300 |
| F | -5.29352600 | -2.11393900 | -1.90730200 |
| F | -4.16574000 | -3.36249600 | 2.47747200 |
| F | 5.00172500 | -2.57965200 | 2.06126100 |
| F | 5.63072600 | -0.73424100 | -2.21054800 |




**R'=H, R=iPr**

Zero-point correction= 0.187629 (Hartree/Particle)
Thermal correction to Energy= 0.196252
Thermal correction to Enthalpy= 0.197196
Thermal correction to Gibbs Free Energy= 0.154015
Sum of electronic and zero-point Energies= -366.424419
Sum of electronic and thermal Energies= -366.415795
Sum of electronic and thermal Enthalpies= -366.414851
Sum of electronic and thermal Free Energies= -366.458032
Single-point electronic energy (M06) = -366.45126

| | | | |
|---|---|---|---|
| C | 1.62104700 | -0.42034000 | 0.00020400 |
| H | 1.72052000 | -1.50866500 | 0.00071900 |
| C | -0.72262200 | -1.25056600 | 0.00033900 |
| C | -0.36985600 | 1.07151300 | -0.00035000 |
| C | -2.09675600 | -1.07152900 | 0.00029400 |
| C | -1.73397500 | 1.30756900 | -0.00041500 |
| C | -2.61547200 | 0.22389800 | -0.00012700 |
| H | -2.74270100 | -1.94229700 | 0.00055900 |
| H | -2.09320500 | 2.33051900 | -0.00067500 |
| N | 0.11934400 | -0.19124400 | -0.00002400 |
| C | 2.24072600 | 0.13607300 | -1.28328700 |
| H | 2.18829800 | 1.22899900 | -1.32638700 |
| H | 3.29854400 | -0.14166800 | -1.30874900 |
| H | 1.76028100 | -0.27631600 | -2.17558400 |
| C | 2.24033900 | 0.13738600 | 1.28331300 |
| H | 3.29828600 | -0.13982500 | 1.30916000 |
| H | 2.18730600 | 1.23032600 | 1.32545300 |
| H | 1.75993600 | -0.27446500 | 2.17588100 |
| H | -0.26301700 | -2.23158800 | 0.00070100 |
| H | 0.35819900 | 1.87229700 | -0.00057600 |
| H | -3.68844300 | 0.38737000 | -0.00015800 |

**R'=Me, R=iPr**

Zero-point correction= 0.244505 (Hartree/Particle)
Thermal correction to Energy= 0.255900
Thermal correction to Enthalpy= 0.256845
Thermal correction to Gibbs Free Energy= 0.208319
Sum of electronic and zero-point Energies= -445.000191

Sum of electronic and thermal Energies= -444.988796
Sum of electronic and thermal Enthalpies= -444.987852
Sum of electronic and thermal Free Energies= -445.036377
Single-point electronic energy (M06) = -445.03993666

| | | | |
|---|---|---|---|
| C | -1.51133500 | 0.57047100 | 0.08059200 |
| H | -1.43476500 | 1.61302000 | 0.36859200 |
| C | 0.92084000 | 1.08497900 | 0.07546100 |
| C | 0.28576900 | -1.22103900 | -0.03737600 |
| C | 2.26179400 | 0.71847100 | 0.04268200 |
| C | 1.63143000 | -1.57978200 | -0.07395800 |
| C | 2.63081500 | -0.61863500 | -0.02631000 |
| H | 3.01132600 | 1.50054600 | 0.06842500 |
| H | 1.87835300 | -2.63291600 | -0.14211100 |
| N | -0.05411900 | 0.10877900 | 0.05078600 |
| C | -2.12584200 | 0.53626600 | -1.32365200 |
| H | -2.26369900 | -0.47555400 | -1.71141100 |
| H | -3.11192100 | 1.00935900 | -1.27983800 |
| H | -1.51610800 | 1.09602700 | -2.03988800 |
| C | -2.35973100 | -0.08875800 | 1.17644800 |
| H | -3.20941600 | 0.57371000 | 1.36963800 |
| H | -2.76886600 | -1.05959200 | 0.89807500 |
| H | -1.80389700 | -0.18756300 | 2.11433200 |
| H | 3.67750300 | -0.90500600 | -0.05185300 |
| C | 0.57056000 | 2.55042000 | 0.13437400 |
| H | -0.07257000 | 2.86240400 | -0.69472800 |
| H | 0.07541600 | 2.82143800 | 1.07399900 |
| H | 1.49051600 | 3.13434700 | 0.07302600 |
| C | -0.73880400 | -2.32379000 | -0.07529900 |
| H | -1.11444000 | -2.54554900 | 0.92896300 |
| H | -1.59140800 | -2.10760000 | -0.71742500 |
| H | -0.26017000 | -3.23014500 | -0.45107300 |

**R'=Ph, R=iPr**

Zero-point correction= 0.349475 (Hartree/Particle)
Thermal correction to Energy= 0.367456
Thermal correction to Enthalpy= 0.368400
Thermal correction to Gibbs Free Energy= 0.302538
Sum of electronic and zero-point Energies= -828.369655
Sum of electronic and thermal Energies= -828.351674
Sum of electronic and thermal Enthalpies= -828.350730
Sum of electronic and thermal Free Energies= -828.416592
Single-point electronic energy (M06) = -828.30120941

| | | | |
|---|---|---|---|
| C | -0.14094100 | -1.15603900 | 0.63460200 |
| H | -1.20649600 | -1.27325400 | 0.81190800 |
| C | -1.26314000 | 0.92554300 | -0.14643800 |
| C | 1.12890500 | 0.91958900 | -0.12835200 |
| C | -1.26032400 | 2.29563500 | -0.40185100 |
| C | 1.12613400 | 2.29106000 | -0.37872800 |
| C | -0.06548600 | 2.99662100 | -0.49377700 |
| H | -2.21520700 | 2.78743400 | -0.54436900 |
| H | 2.08399200 | 2.78211300 | -0.50341700 |
| N | -0.06806700 | 0.25856700 | 0.04078100 |
| C | -2.57446400 | 0.22350200 | -0.09508600 |
| C | -3.52406600 | 0.61195000 | 0.86376800 |
| C | -2.91811100 | -0.74074100 | -1.05875700 |
| C | -4.78762200 | 0.02219200 | 0.87562700 |
| H | -3.26805600 | 1.36267000 | 1.60632300 |
| C | -4.18669100 | -1.31662700 | -1.04772900 |
| H | -2.20530200 | -1.01877900 | -1.82962500 |
| C | -5.12024600 | -0.94095500 | -0.07856100 |
| H | -5.51180300 | 0.31897900 | 1.62803200 |
| H | -4.44882600 | -2.05235000 | -1.80189700 |
| H | -6.10719800 | -1.39344300 | -0.07212600 |
| C | 2.45730900 | 0.24101400 | -0.09524800 |
| C | 2.88096900 | -0.53995800 | -1.18181600 |
| C | 3.36227700 | 0.53584900 | 0.93703600 |
| C | 4.17792300 | -1.05304200 | -1.21077000 |
| H | 2.20841100 | -0.72609100 | -2.01371500 |
| C | 4.65329900 | 0.00994400 | 0.90818200 |
| H | 3.05123500 | 1.16512700 | 1.76642900 |
| C | 5.06168900 | -0.78706300 | -0.16341300 |
| H | 4.49898400 | -1.65136700 | -2.05800600 |
| H | 5.34115400 | 0.23049200 | 1.71871000 |
| H | 6.07011400 | -1.18868900 | -0.18838500 |
| C | 0.28282900 | -2.26947600 | -0.32592600 |
| H | 1.36562000 | -2.36993800 | -0.40094700 |
| H | -0.11607300 | -3.21193200 | 0.06382900 |
| H | -0.13120100 | -2.12576900 | -1.32822900 |
| C | 0.54714600 | -1.22301900 | 2.00130000 |
| H | 0.24385600 | -2.16188200 | 2.47631200 |
| H | 1.63544100 | -1.22014100 | 1.93378100 |
| H | 0.22479500 | -0.40394600 | 2.65243400 |
| H | -0.06130500 | 4.06491300 | -0.68689500 |

**R'=CF3, R=iPr**

Zero-point correction= 0.197608 (Hartree/Particle)
Thermal correction to Energy= 0.212919
Thermal correction to Enthalpy= 0.213863
Thermal correction to Gibbs Free Energy= 0.155269
Sum of electronic and zero-point Energies= -1040.434091
Sum of electronic and thermal Energies= -1040.418780
Sum of electronic and thermal Enthalpies= -1040.417836
Sum of electronic and thermal Free Energies= -1040.476430
Single-point electronic energy (M06) = -1040.45563053

| | | | |
|---|---|---|---|
| C | -0.10509600 | -1.56761400 | -0.03604100 |
| H | -1.12617200 | -1.77115800 | 0.24831800 |
| C | -1.25262700 | 0.67234100 | 0.00183600 |
| C | 1.10041700 | 0.73391900 | -0.06585600 |
| C | -1.31456400 | 2.05747800 | -0.07043500 |
| C | 1.06492400 | 2.12356700 | -0.14204000 |
| C | -0.14560500 | 2.80101500 | -0.15327200 |
| H | -2.28313100 | 2.53827400 | -0.06037000 |
| H | 2.00038300 | 2.66345300 | -0.18910100 |
| N | -0.05569800 | -0.00159600 | -0.00343700 |
| C | 0.08133800 | -2.06085300 | -1.47377200 |
| H | 1.08361800 | -1.88725100 | -1.86097200 |
| H | -0.09763200 | -3.14112000 | -1.47203100 |
| H | -0.65139400 | -1.60656200 | -2.14539200 |
| C | 0.74327200 | -2.25930300 | 1.03377000 |
| H | 0.32720900 | -3.26691300 | 1.13630100 |
| H | 1.79368000 | -2.36727400 | 0.77717100 |
| H | 0.64950600 | -1.77010300 | 2.00705300 |
| H | -0.17654400 | 3.88385100 | -0.21654200 |
| C | -2.60268700 | -0.06816800 | 0.10422200 |
| C | 2.51628300 | 0.12671900 | 0.04966300 |
| F | 3.41991600 | 1.04982200 | -0.30139300 |
| F | 2.71273100 | -0.93697700 | -0.73786800 |
| F | 2.74995400 | -0.21645700 | 1.32377400 |
| F | -3.60180000 | 0.81688600 | 0.10313300 |
| F | -2.67570700 | -0.77135800 | 1.24687500 |
| F | -2.78771200 | -0.89954200 | -0.93327900 |

**R'=Cl, R=iPr**

Zero-point correction= 0.167769 (Hartree/Particle)
Thermal correction to Energy= 0.178798
Thermal correction to Enthalpy= 0.179742
Thermal correction to Gibbs Free Energy= 0.129988
Sum of electronic and zero-point Energies= -1285.598651
Sum of electronic and thermal Energies= -1285.587622
Sum of electronic and thermal Enthalpies= -1285.586678
Sum of electronic and thermal Free Energies= -1285.636432
Single-point electronic energy (M06) = -1285.60750590

| | | | |
|---|---|---|---|
| C | 0.35944200 | -1.57454800 | -0.00000200 |
| H | -0.59527600 | -2.08780100 | 0.00000000 |
| C | -1.40101500 | 0.24703000 | 0.00003000 |
| C | 0.84454000 | 0.94267500 | 0.00006400 |
| C | -1.83394300 | 1.56597100 | 0.00000600 |
| C | 0.45255900 | 2.27534200 | 0.00001800 |
| C | -0.89932500 | 2.59384400 | 0.00000000 |
| H | -2.89881800 | 1.76321000 | -0.00002900 |
| H | 1.21957700 | 3.04003900 | -0.00001100 |
| N | -0.06514900 | -0.08503400 | 0.00005300 |
| C | 1.06706400 | -1.96253000 | -1.30132800 |
| H | 2.08880200 | -1.59118300 | -1.37695500 |
| H | 1.10891100 | -3.05626300 | -1.32920100 |

| | | | |
|---|---|---|---|
| H | 0.49911600 | -1.63272900 | -2.17673300 |
| C | 1.06711100 | -1.96266700 | 1.30126000 |
| H | 1.10879900 | -3.05640800 | 1.32907300 |
| H | 2.08890700 | -1.59147600 | 1.37684700 |
| H | 0.49926500 | -1.63283500 | 2.17672100 |
| H | -1.22096800 | 3.63042300 | -0.00003600 |
| Cl | 2.53571300 | 0.62721800 | -0.00001100 |
| Cl | -2.61694000 | -0.97665600 | -0.00001000 |

**R'=tBu, R=iPr**

Zero-point correction= 0.415506 (Hartree/Particle)
Thermal correction to Energy= 0.434517
Thermal correction to Enthalpy= 0.435461
Thermal correction to Gibbs Free Energy= 0.371382
Sum of electronic and zero-point Energies= -680.662476
Sum of electronic and thermal Energies= -680.643465
Sum of electronic and thermal Enthalpies= -680.642520
Sum of electronic and thermal Free Energies= -680.706599
Single-point electronic energy (M06) = -680.75017227

| | | | |
|---|---|---|---|
| C | -0.13680500 | -1.52032800 | 0.57768600 |
| H | -1.20620100 | -1.66420300 | 0.60546600 |
| C | -1.25385600 | 0.62485200 | 0.10146600 |
| C | 1.17181400 | 0.66430700 | 0.15103400 |
| C | -1.27023500 | 1.97010100 | 0.46692800 |
| C | 1.11041100 | 1.99841400 | 0.54133000 |
| C | -0.09934900 | 2.63552000 | 0.78284600 |
| H | -2.21230000 | 2.49456100 | 0.51600100 |
| H | 2.02622000 | 2.55789000 | 0.64938300 |
| N | -0.03494300 | -0.04579200 | 0.11577300 |
| C | 0.39475900 | -2.64056300 | -0.31856100 |
| H | 1.47661200 | -2.74428400 | -0.33706100 |
| H | -0.01023300 | -3.57442400 | 0.08756100 |
| H | 0.03297300 | -2.55161700 | -1.34465300 |
| C | 0.31476500 | -1.59334700 | 2.04465300 |
| H | 0.08696700 | -2.59616300 | 2.42092200 |
| H | 1.38047100 | -1.41832000 | 2.18586900 |
| H | -0.23899600 | -0.87373300 | 2.65589200 |
| H | -0.12197700 | 3.66035600 | 1.14057900 |
| C | -2.60780500 | -0.02387100 | -0.33651200 |
| C | 2.53637700 | 0.11747300 | -0.37503800 |
| C | -3.48421500 | 1.08652800 | -0.99077600 |
| H | -4.36444200 | 0.61104800 | -1.43125500 |
| H | -3.85897300 | 1.81942900 | -0.27185000 |
| H | -2.95424300 | 1.61469300 | -1.79005900 |
| C | -3.40931900 | -0.56181000 | 0.87880000 |
| H | -2.93917900 | -1.41587500 | 1.37628700 |
| H | -3.56036900 | 0.22075600 | 1.62964800 |
| H | -4.39577800 | -0.89052200 | 0.53613200 |
| C | -2.44813600 | -1.11442200 | -1.42908400 |
| H | -1.76172900 | -0.79355400 | -2.22004700 |
| H | -2.11842600 | -2.08364200 | -1.05405000 |
| H | -3.42328100 | -1.28469300 | -1.89327100 |
| C | 2.31881000 | -0.42789100 | -1.81266000 |
| H | 1.58620600 | -1.22812100 | -1.87734700 |
| H | 1.99563500 | 0.37792600 | -2.48073400 |
| H | 3.26962300 | -0.81262800 | -2.19515600 |
| C | 3.26070000 | -0.89723200 | 0.54455700 |
| H | 3.41723800 | -0.47347400 | 1.54241200 |
| H | 2.75905100 | -1.85498000 | 0.65623600 |
| H | 4.24796000 | -1.10283500 | 0.11953300 |
| C | 3.54581100 | 1.28810900 | -0.53691400 |
| H | 3.15774900 | 2.09665200 | -1.16374300 |
| H | 3.87513300 | 1.70191800 | 0.42176100 |
| H | 4.43651700 | 0.89333300 | -1.03338800 |

**R'=H, R=Et**

Zero-point correction= 0.159686 (Hartree/Particle)
Thermal correction to Energy= 0.166904
Thermal correction to Enthalpy= 0.167848
Thermal correction to Gibbs Free Energy= 0.127795
Sum of electronic and zero-point Energies= -327.134949
Sum of electronic and thermal Energies= -327.127731
Sum of electronic and thermal Enthalpies= -327.126787
Sum of electronic and thermal Free Energies= -327.166841
Single-point electronic energy (M06) = -327.15652389

| | | | |
|---|---|---|---|
| C | -1.87767400 | -0.00001200 | -0.58172100 |
| H | -2.08811300 | 0.88200600 | -1.19042900 |
| C | 0.25323100 | 1.17700000 | -0.18319200 |
| C | 0.25324200 | -1.17700700 | -0.18318400 |
| C | 1.60836300 | 1.20487100 | 0.10036900 |
| C | 1.60837200 | -1.20486300 | 0.10037800 |
| C | 2.29995400 | 0.00000800 | 0.24479900 |
| H | 2.10790100 | 2.16186400 | 0.20088100 |
| H | 2.10792000 | -2.16185100 | 0.20089700 |
| N | -0.40170300 | -0.00000600 | -0.32205900 |
| C | -2.68159800 | 0.00001000 | 0.71626200 |
| H | -3.74745600 | -0.00001400 | 0.46933900 |
| H | -2.47320600 | -0.88951800 | 1.31879400 |
| H | -2.47323700 | 0.88957500 | 1.31874900 |
| H | 3.36296900 | 0.00001200 | 0.46370400 |
| H | -2.08811300 | -0.88205200 | -1.19039600 |
| H | -0.34003500 | -2.07506000 | -0.30969300 |
| H | -0.34005200 | 2.07504700 | -0.30970700 |

**R'=Me, R=Et**

Zero-point correction= 0.216267 (Hartree/Particle)
Thermal correction to Energy= 0.226207
Thermal correction to Enthalpy= 0.227151
Thermal correction to Gibbs Free Energy= 0.181907
Sum of electronic and zero-point Energies= -405.721663
Sum of electronic and thermal Energies= -405.711723
Sum of electronic and thermal Enthalpies= -405.710779
Sum of electronic and thermal Free Energies= -405.756023
Single-point electronic energy (M06) = -405.75481765

| | | | |
|---|---|---|---|
| C | 1.76138500 | 0.00013300 | -0.46706700 |
| H | 1.99272000 | 0.87375600 | -1.07385200 |
| C | -0.37454700 | 1.20042900 | -0.10641300 |
| C | -0.37444000 | -1.20048000 | -0.10650500 |
| C | -1.73985700 | 1.19837200 | 0.15791400 |
| C | -1.73975400 | -1.19856800 | 0.15779700 |
| C | -2.43177300 | -0.00013700 | 0.29395900 |
| H | -2.25024200 | 2.14970300 | 0.25324700 |
| H | -2.25002900 | -2.14997100 | 0.25299000 |
| N | 0.28165100 | -0.00001700 | -0.22984200 |
| C | 2.56391000 | 0.00010900 | 0.83554800 |
| H | 2.35650800 | -0.88481100 | 1.44378000 |
| H | 3.63049900 | 0.00004100 | 0.59117500 |
| H | 2.35648400 | 0.88519900 | 1.44351400 |
| H | -3.49723200 | -0.00018900 | 0.50160500 |
| C | 0.36752600 | 2.49703100 | -0.27939700 |
| H | 1.24107200 | 2.57446200 | 0.37390100 |
| H | 0.70617600 | 2.63005900 | -1.31423300 |
| H | -0.30039600 | 3.32724400 | -0.04409900 |
| C | 0.36785500 | -2.49698100 | -0.27936300 |
| H | 0.70807300 | -2.62951700 | -1.31370700 |
| H | 1.24047400 | -2.57459900 | 0.37521100 |
| H | -0.30030700 | -3.32737500 | -0.04540400 |
| H | 1.99280800 | -0.87332200 | -1.07406700 |

**R'=Ph, R=Et**

Zero-point correction= 0.321466 (Hartree/Particle)
Thermal correction to Energy= 0.338017
Thermal correction to Enthalpy= 0.338961
Thermal correction to Gibbs Free Energy= 0.276033
Sum of electronic and zero-point Energies= -789.091504
Sum of electronic and thermal Energies= -789.074953
Sum of electronic and thermal Enthalpies= -789.074009
Sum of electronic and thermal Free Energies= -789.136937
Single-point electronic energy (M06) = -789.01510770

| | | | |
|---|---|---|---|
| C | 0.00000900 | -1.25458800 | 0.38879000 |
| H | -0.88036200 | -1.72917800 | -0.03413700 |
| C | -1.19980500 | 0.84868400 | -0.16887700 |
| C | 1.19975800 | 0.84862600 | -0.16900400 |
| C | -1.19779500 | 2.23342100 | -0.32327900 |

| | | | |
|---|---|---|---|
| C | 1.19784600 | 2.23342500 | -0.32333600 |
| C | 0.00005200 | 2.93731100 | -0.38217000 |
| H | -2.15262300 | 2.73724300 | -0.41590700 |
| H | 2.15271900 | 2.73716300 | -0.41594500 |
| N | 0.00002200 | 0.18329800 | -0.06077700 |
| C | -2.49657800 | 0.12128800 | -0.13186700 |
| C | -3.41709800 | 0.40849800 | 0.88754200 |
| C | -2.85348600 | -0.77026200 | -1.15849100 |
| C | -4.66699100 | -0.21139400 | 0.89540700 |
| H | -3.15177800 | 1.10669900 | 1.67674000 |
| C | -4.10746900 | -1.37717800 | -1.14942700 |
| H | -2.16279500 | -0.96784700 | -1.97432700 |
| C | -5.01265900 | -1.10355300 | -0.12051700 |
| H | -5.36983800 | 0.00729200 | 1.69339700 |
| H | -4.38112700 | -2.05639700 | -1.95097400 |
| H | -5.98833100 | -1.57984200 | -0.11614600 |
| C | 2.49657900 | 0.12127200 | -0.13193300 |
| C | 2.85347900 | -0.77035700 | -1.15849200 |
| C | 3.41705600 | 0.40856400 | 0.88747200 |
| C | 4.10746400 | -1.37725800 | -1.14936700 |
| H | 2.16281200 | -0.96795600 | -1.97434200 |
| C | 4.66695500 | -0.21133900 | 0.89540900 |
| H | 3.15172800 | 1.10683800 | 1.67660300 |
| C | 5.01263000 | -1.10356900 | -0.12043900 |
| H | 4.38115400 | -2.05653500 | -1.95085300 |
| H | 5.36981900 | 0.00742900 | 1.69336200 |
| H | 5.98830300 | -1.57985600 | -0.11600700 |
| C | 0.00000200 | -1.34502100 | 1.91342100 |
| H | -0.00043800 | -2.40093400 | 2.20143500 |
| H | 0.89122900 | -0.87725800 | 2.34189400 |
| H | -0.89082100 | -0.87658200 | 2.34200600 |
| H | 0.00002400 | 4.01631100 | -0.50238300 |
| H | 0.88047100 | -1.72910300 | -0.03403300 |

**R'=CF3, R=Et**

Zero-point correction= 0.169566 (Hartree/Particle)
Thermal correction to Energy= 0.183430
Thermal correction to Enthalpy= 0.184374
Thermal correction to Gibbs Free Energy= 0.128701
Sum of electronic and zero-point Energies= -1001.157037
Sum of electronic and thermal Energies= -1001.143173
Sum of electronic and thermal Enthalpies= -1001.142229
Sum of electronic and thermal Free Energies= -1001.197902
Single-point electronic energy (M06) = -1001.17246354

| | | | |
|---|---|---|---|
| C | 0.00014900 | -1.61362500 | 0.19921400 |
| H | -0.87289200 | -1.86313100 | 0.79443800 |
| C | -1.17927200 | 0.58688400 | -0.05414400 |
| C | 1.17921900 | 0.58698300 | -0.05412600 |
| C | -1.19671700 | 1.94958100 | -0.31923100 |
| C | 1.19657300 | 1.94968200 | -0.31919900 |
| C | -0.00009900 | 2.64116900 | -0.47513000 |
| H | -2.15049200 | 2.45520100 | -0.39295100 |
| H | 2.15031000 | 2.45537300 | -0.39290900 |
| N | 0.00000700 | -0.09723900 | 0.04651900 |
| C | 0.00030800 | -2.33461000 | -1.14889800 |
| H | 0.89106500 | -2.10515100 | -1.73451200 |
| H | 0.00043700 | -3.40986700 | -0.94235300 |
| H | -0.89045000 | -2.10537900 | -1.73459600 |
| H | -0.00014000 | 3.70445500 | -0.69215800 |
| C | -2.52401200 | -0.12155500 | 0.18987400 |
| C | 2.52396500 | -0.12143400 | 0.18990000 |
| H | 0.87321900 | -1.86292100 | 0.79449500 |
| F | -3.51968300 | 0.75763200 | 0.06644100 |
| F | -2.55787600 | -0.62627000 | 1.43472400 |
| F | -2.73169700 | -1.11632000 | -0.68313600 |
| F | 2.55772400 | -0.62627900 | 1.43469600 |
| F | 2.73169300 | -1.11613000 | -0.68317700 |
| F | 3.51964000 | 0.75777200 | 0.06660300 |

**R'=Cl, R=Et**

Zero-point correction= 0.140062 (Hartree/Particle)
Thermal correction to Energy= 0.149424
Thermal correction to Enthalpy= 0.150368
Thermal correction to Gibbs Free Energy= 0.104704
Sum of electronic and zero-point Energies= -1246.317941
Sum of electronic and thermal Energies= -1246.308580
Sum of electronic and thermal Enthalpies= -1246.307635
Sum of electronic and thermal Free Energies= -1246.353299
Single-point electronic energy (M06) = -1246.32123574

| | | | |
|---|---|---|---|
| C | 0.00007600 | -1.69971600 | -0.44902900 |
| H | -0.87842700 | -1.90745800 | -1.05637400 |
| C | -1.18001500 | 0.47635300 | -0.06483800 |
| C | 1.18003500 | 0.47646000 | -0.06496800 |
| C | -1.20225000 | 1.84455000 | 0.16478900 |
| C | 1.20216100 | 1.84463900 | 0.16466900 |
| C | -0.00007400 | 2.53590800 | 0.27670900 |
| H | -2.15939000 | 2.34367500 | 0.25423900 |
| H | 2.15925400 | 2.34388200 | 0.25397100 |
| N | 0.00003100 | -0.21053800 | -0.19471500 |
| C | 0.00003100 | -2.50231000 | 0.84966700 |
| H | 0.00040000 | -3.56608300 | 0.59247600 |
| H | 0.89031200 | -2.30066700 | 1.45140000 |
| H | -0.89061500 | -2.30106700 | 1.45096600 |
| H | -0.00008900 | 3.60645200 | 0.45569500 |
| Cl | 2.66956800 | -0.37328900 | -0.18364800 |
| Cl | -2.66957300 | -0.37335100 | -0.18370800 |
| H | 0.87864800 | -1.90739100 | -1.05630600 |

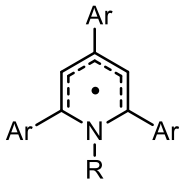
**R'=tBu, R=Et**

Zero-point correction= 0.387499 (Hartree/Particle)
Thermal correction to Energy= 0.405072
Thermal correction to Enthalpy= 0.406016
Thermal correction to Gibbs Free Energy= 0.344964
Sum of electronic and zero-point Energies= -641.397653
Sum of electronic and thermal Energies= -641.380080
Sum of electronic and thermal Enthalpies= -641.379136
Sum of electronic and thermal Free Energies= -641.440188
Single-point electronic energy (M06) = -641.47587946

| | | | |
|---|---|---|---|
| C | 0.00000600 | -1.63743400 | -0.16220100 |
| H | 0.86865300 | -2.01096900 | 0.36230200 |
| C | 1.21831900 | 0.52161500 | -0.14740800 |
| C | -1.21831700 | 0.52160500 | -0.14742900 |
| C | 1.19646500 | 1.84943900 | -0.56728500 |
| C | -1.19642100 | 1.84950000 | -0.56711000 |
| C | 0.00001900 | 2.49625900 | -0.83945700 |
| H | 2.12511500 | 2.38618100 | -0.68125400 |
| H | -2.12505700 | 2.38629000 | -0.68094300 |
| N | -0.00001300 | -0.14098000 | -0.06987200 |
| C | 0.00001700 | -2.09251400 | -1.62369500 |
| H | -0.00002100 | -3.18739200 | -1.65108300 |
| H | -0.88548100 | -1.74058400 | -2.15770000 |
| H | 0.88559100 | -1.74065200 | -2.15761800 |
| H | 0.00002600 | 3.51760800 | -1.20786400 |
| C | 2.56294200 | -0.11438600 | 0.32221700 |
| C | -2.56297100 | -0.11437100 | 0.32219100 |
| C | 3.67155500 | 0.97110700 | 0.34830700 |
| H | 4.57416000 | 0.52305700 | 0.77230200 |
| H | 3.93315200 | 1.32918100 | -0.65278200 |
| H | 3.40901500 | 1.82671500 | 0.97815800 |
| C | 3.11377000 | -1.23597700 | -0.60066500 |
| H | 2.55285000 | -2.17076000 | -0.57257800 |
| H | 3.16808900 | -0.89744200 | -1.64077900 |
| H | 4.13338700 | -1.47149300 | -0.28120800 |
| C | 2.41717400 | -0.59459400 | 1.79404400 |
| H | 2.15204900 | 0.24273300 | 2.44807600 |
| H | 1.67713100 | -1.38299900 | 1.94816500 |
| H | 3.38104600 | -0.98775200 | 2.13158600 |
| C | -2.41710300 | -0.59455800 | 1.79400900 |
| H | -1.67724000 | -1.38316200 | 1.94801400 |
| H | -2.15166800 | 0.24271200 | 2.44799000 |
| H | -3.38102300 | -0.98746700 | 2.13171400 |
| C | -3.11386200 | -1.23600700 | -0.60060800 |
| H | -3.16811400 | -0.89758500 | -1.64076200 |
| H | -2.55308800 | -2.17086500 | -0.57238400 |

| | | | |
|---|---|---|---|
| H | -4.13351500 | -1.47135500 | -0.28115000 |
| C | -3.67157600 | 0.97111900 | 0.34826100 |
| H | -3.40899800 | 1.82683200 | 0.97796400 |
| H | -3.93330200 | 1.32904000 | -0.65284800 |
| H | -4.57411500 | 0.52312400 | 0.77246000 |
| H | -0.86865700 | -2.01095500 | 0.36230600 |

## Pyridinium radicals




**Ar=Ph, R=Cy**

Zero-point correction= 0.493613 (Hartree/Particle)
Thermal correction to Energy= 0.518218
Thermal correction to Enthalpy= 0.519162
Thermal correction to Gibbs Free Energy= 0.437355
Sum of electronic and zero-point Energies= -1176.191556
Sum of electronic and thermal Energies= -1176.166951
Sum of electronic and thermal Enthalpies= -1176.166007
Sum of electronic and thermal Free Energies= -1176.247814
Single-point electronic energy (M06) = -1176.07158133

| | | | |
|---|---|---|---|
| C | 0.17309700 | 1.30534000 | -0.31389300 |
| C | -0.00909000 | -1.09951600 | -0.37844000 |
| C | 1.53844600 | 1.19165900 | -0.19956300 |
| C | 1.35317600 | -1.19532000 | -0.23973500 |
| C | 2.19257000 | -0.05969900 | -0.06039200 |
| H | 2.12208800 | 2.10272600 | -0.27019600 |
| H | 1.80412500 | -2.16829300 | -0.40635600 |
| N | -0.66072500 | 0.15530900 | -0.23771800 |
| C | -0.47313500 | 2.60498700 | -0.58352400 |
| C | 0.02007900 | 3.79666000 | -0.01669400 |
| C | -1.58732100 | 2.69417100 | -1.44193200 |
| C | -0.56339800 | 5.02623900 | -0.31247800 |
| H | 0.85353600 | 3.75062000 | 0.67856000 |
| C | -2.17063200 | 3.92476200 | -1.73307400 |
| H | -1.97481700 | 1.78724100 | -1.89587000 |
| C | -1.66210000 | 5.09899400 | -1.17217900 |
| H | -0.16624600 | 5.93054900 | 0.14146200 |
| H | -3.02194800 | 3.96821000 | -2.40773600 |
| C | -0.79933300 | -2.27560000 | -0.80642300 |
| C | -1.70331000 | -2.18437900 | -1.88166200 |
| C | -0.60754200 | -3.53211500 | -0.20454200 |
| C | -2.38694100 | -3.30870900 | -2.33683800 |
| H | -1.85107900 | -1.22343500 | -2.36513900 |
| C | -1.29390000 | -4.65701300 | -0.66088700 |
| H | 0.07609500 | -3.61808300 | 0.63583900 |
| C | -2.18753100 | -4.55130100 | -1.72807700 |
| H | -3.07216800 | -3.21770300 | -3.17581400 |
| H | -1.13500200 | -5.61671600 | -0.17589600 |
| C | 3.64023800 | -0.18782400 | 0.12638500 |
| C | 4.19820400 | -1.37058800 | 0.66147900 |
| C | 4.53611200 | 0.85182800 | -0.20883500 |
| C | 5.57093000 | -1.50713300 | 0.84565800 |
| H | 3.54143400 | -2.18074900 | 0.96453100 |
| C | 5.90790300 | 0.71422100 | -0.02052600 |
| H | 4.15828700 | 1.76872200 | -0.65098900 |
| C | 6.43861400 | -0.46597400 | 0.50722800 |
| H | 5.96469800 | -2.42918900 | 1.26623900 |
| H | 6.56924200 | 1.53148300 | -0.29770400 |
| C | -1.77329600 | 0.26950800 | 0.77820000 |
| C | -3.13889200 | -0.28222500 | 0.34208600 |
| C | -1.35526800 | -0.30484400 | 2.14512700 |
| H | -1.90199000 | 1.34798000 | 0.90492800 |
| C | -4.20192500 | 0.04112600 | 1.40804700 |
| H | -3.08982400 | -1.36638900 | 0.20495600 |
| H | -3.42381000 | 0.15136400 | -0.62381300 |
| C | -2.42210900 | -0.00791500 | 3.21232800 |
| H | -1.21679200 | -1.39058200 | 2.05804000 |
| H | -0.38796200 | 0.11907700 | 2.44078300 |
| C | -3.80670300 | -0.51556500 | 2.78431900 |
| H | -5.17125700 | -0.36694900 | 1.09574500 |
| H | -4.33070500 | 1.13132800 | 1.47940300 |
| H | -2.12716800 | -0.45927600 | 4.16809300 |
| H | -2.47123600 | 1.07760100 | 3.38303100 |
| H | -4.55965700 | -0.24452200 | 3.53521400 |
| H | -3.79087300 | -1.61431100 | 2.73731000 |
| H | -2.72390000 | -5.42720500 | -2.08266700 |
| H | 7.51007100 | -0.57155200 | 0.65291300 |
| H | -2.11973200 | 6.05823000 | -1.39782200 |

**Ar=4-Me-Ph, R=Cy**

Zero-point correction= 0.576132 (Hartree/Particle)
Thermal correction to Energy= 0.606473
Thermal correction to Enthalpy= 0.607417
Thermal correction to Gibbs Free Energy= 0.510928
Sum of electronic and zero-point Energies= -1294.063245
Sum of electronic and thermal Energies= -1294.032903
Sum of electronic and thermal Enthalpies= -1294.031959
Sum of electronic and thermal Free Energies= -1294.128448
Single-point electronic energy (M06) = -1293.95598718

| | | | |
|---|---|---|---|
| C | 0.01789200 | 1.30262200 | -0.22059800 |
| C | -0.06022900 | -1.10960600 | -0.23484800 |
| C | 1.39113900 | 1.25104400 | -0.18760200 |
| C | 1.31116800 | -1.14162600 | -0.17842900 |
| C | 2.10892900 | 0.03239100 | -0.07113700 |
| H | 1.92663200 | 2.18636300 | -0.30718900 |
| H | 1.79423300 | -2.09731700 | -0.35478900 |
| N | -0.75837900 | 0.11860200 | -0.07947400 |
| C | -0.69887800 | 2.56904800 | -0.46622900 |
| C | -0.23813200 | 3.78760200 | 0.06726600 |
| C | -1.85735700 | 2.60820700 | -1.26656900 |
| C | -0.89377600 | 4.98508000 | -0.20424500 |
| H | 0.62768400 | 3.78881800 | 0.72359700 |
| C | -2.50852200 | 3.80918600 | -1.53004300 |
| H | -2.23128100 | 1.68462600 | -1.69784300 |
| C | -2.04004000 | 5.02396500 | -1.00961400 |
| H | -0.51583600 | 5.90783400 | 0.23110500 |
| H | -3.39617700 | 3.80518800 | -2.15948600 |
| C | -0.81960700 | -2.32998100 | -0.58503700 |
| C | -1.79768400 | -2.31358100 | -1.59739500 |
| C | -0.52702500 | -3.56453800 | 0.01853300 |
| C | -2.44847800 | -3.48015300 | -1.98338900 |
| H | -2.02787800 | -1.37507500 | -2.09280400 |
| C | -1.18447600 | -4.73007400 | -0.37276100 |
| H | 0.21735900 | -3.60566900 | 0.80934100 |
| C | -2.15969400 | -4.71267000 | -1.37666600 |
| H | -3.18946600 | -3.43797800 | -2.77931400 |
| H | -0.93882600 | -5.66989200 | 0.11709900 |
| C | 3.56911000 | -0.02929800 | 0.01970000 |
| C | 4.22028400 | -1.17527600 | 0.52547500 |
| C | 4.39736900 | 1.04249400 | -0.38136700 |
| C | 5.60693000 | -1.24511400 | 0.61557300 |
| H | 3.62855500 | -2.01203900 | 0.88525100 |
| C | 5.78164000 | 0.96605000 | -0.28526400 |
| H | 3.95475400 | 1.94093200 | -0.80078500 |
| C | 6.42141200 | -0.17971200 | 0.21075000 |
| H | 6.06713000 | -2.14434800 | 1.02046200 |
| H | 6.38215500 | 1.81299400 | -0.61200900 |
| C | -1.82856400 | 0.20325200 | 0.98260700 |
| C | -3.20499500 | -0.35585500 | 0.58983600 |
| C | -1.35525100 | -0.38564100 | 2.32504800 |
| H | -1.96401000 | 1.27801000 | 1.13239300 |
| C | -4.23175200 | -0.05524500 | 1.69650600 |
| H | -3.15036500 | -1.43784400 | 0.43757200 |
| H | -3.52863000 | 0.08674700 | -0.35956000 |
| C | -2.38637900 | -0.11257600 | 3.43355800 |
| H | -1.20929400 | -1.46854100 | 2.21987900 |

| | | | |
|---|---|---|---|
| H | -0.38248000 | 0.04514800 | 2.59145400 |
| C | -3.78205100 | -0.62644800 | 3.04950400 |
| H | -5.20873400 | -0.46736800 | 1.41452900 |
| H | -4.36639800 | 1.03288200 | 1.78686300 |
| H | -2.05347000 | -0.57352300 | 4.37217900 |
| H | -2.43857200 | 0.97023600 | 3.62015400 |
| H | -4.50869500 | -0.37180500 | 3.83151900 |
| H | -3.75909200 | -1.72432000 | 2.98708100 |
| C | -2.89343000 | -5.96884600 | -1.78289100 |
| H | -3.00154700 | -6.03604100 | -2.87169000 |
| H | -2.36962900 | -6.86718100 | -1.44037600 |
| H | -3.90580300 | -5.99727900 | -1.35762300 |
| C | 7.92726400 | -0.26640600 | 0.28144300 |
| H | 8.36240200 | -0.51863200 | -0.69559600 |
| H | 8.37186900 | 0.68580900 | 0.59343900 |
| H | 8.25103800 | -1.03687900 | 0.98933400 |
| C | -2.73393300 | 6.32837600 | -1.32275800 |
| H | -2.56725800 | 7.07066500 | -0.53476500 |
| H | -2.36383500 | 6.76313300 | -2.26146700 |
| H | -3.81518900 | 6.19209300 | -1.43536900 |

**Ar=4-MeO-Ph, R=Cy**

Zero-point correction= 0.591671 (Hartree/Particle)
Thermal correction to Energy= 0.624203
Thermal correction to Enthalpy= 0.625147
Thermal correction to Gibbs Free Energy= 0.525122
Sum of electronic and zero-point Energies= -1519.660706
Sum of electronic and thermal Energies= -1519.628174
Sum of electronic and thermal Enthalpies= -1519.627230
Sum of electronic and thermal Free Energies= -1519.727255
Single-point electronic energy (M06) = -1519.55551246

| | | | |
|---|---|---|---|
| C | 0.21439900 | -1.31653800 | -0.13807300 |
| C | -0.04874400 | 1.08386000 | -0.12214800 |
| C | -1.15047600 | -1.45798700 | -0.22004700 |
| C | -1.41056700 | 0.92275800 | -0.18264200 |
| C | -2.04007100 | -0.35412800 | -0.14414700 |
| H | -1.53920800 | -2.45375400 | -0.40320600 |
| H | -2.00919600 | 1.80160900 | -0.40139000 |
| N | 0.79934000 | -0.03820100 | 0.09713900 |
| C | 1.12820600 | -2.45556400 | -0.34342200 |
| C | 0.79023700 | -3.75935000 | 0.07996400 |
| C | 2.36154700 | -2.29289400 | -0.99703600 |
| C | 1.62746500 | -4.83804400 | -0.15825100 |
| H | -0.13626000 | -3.92048500 | 0.62361100 |
| C | 3.21552800 | -3.36913900 | -1.23948300 |
| H | 2.64573300 | -1.30372200 | -1.34255200 |
| C | 2.85019300 | -4.65451400 | -0.82233700 |
| H | 1.36407200 | -5.83705700 | 0.17549800 |
| H | 4.15125500 | -3.19525400 | -1.75908300 |
| C | 0.56659900 | 2.39818300 | -0.40187800 |
| C | 1.64645100 | 2.52340600 | -1.28990300 |
| C | 0.03899000 | 3.58393700 | 0.14829800 |
| C | 2.18316400 | 3.76648300 | -1.62436500 |
| H | 2.06395000 | 1.62752900 | -1.73931400 |
| C | 0.56256100 | 4.82787500 | -0.17485000 |
| H | -0.78715300 | 3.52068900 | 0.85136000 |
| C | 1.64079000 | 4.93108000 | -1.06577100 |
| H | 3.00990100 | 3.81549900 | -2.32424400 |
| H | 0.15845200 | 5.73789600 | 0.25794000 |
| C | -3.49693700 | -0.49950600 | -0.15791900 |
| C | -4.33681500 | 0.53133300 | 0.30812100 |
| C | -4.13897400 | -1.67033700 | -0.62761500 |
| C | -5.72698300 | 0.41974600 | 0.30611500 |
| H | -3.89519300 | 1.43753700 | 0.71217300 |
| C | -5.51848100 | -1.79600700 | -0.63212600 |
| H | -3.54709300 | -2.48975100 | -1.02398100 |
| C | -6.33067900 | -0.75083100 | -0.16571500 |
| H | -6.32297400 | 1.24268600 | 0.68492500 |
| H | -5.99711100 | -2.69640500 | -1.00548300 |
| C | 1.71903600 | -0.00268600 | 1.29492500 |
| C | 3.02136900 | 0.79289100 | 1.11457500 |
| C | 0.98046100 | 0.43329300 | 2.57436700 |
| H | 2.01271600 | -1.04746500 | 1.43093400 |
| C | 3.92710600 | 0.60623200 | 2.34532100 |
| H | 2.80641500 | 1.85832500 | 0.98758400 |
| H | 3.53805800 | 0.45833000 | 0.20706600 |
| C | 1.88387800 | 0.27464100 | 3.80890700 |
| H | 0.67202600 | 1.48261100 | 2.47826200 |
| H | 0.06560700 | -0.16037200 | 2.68920700 |
| C | 3.21259800 | 1.02604500 | 3.63882800 |
| H | 4.85035800 | 1.18483100 | 2.21519200 |
| H | 4.22836700 | -0.44913400 | 2.42209300 |
| H | 1.35649700 | 0.62778200 | 4.70420100 |
| H | 2.09078700 | -0.79356900 | 3.97080100 |
| H | 3.86168100 | 0.85176500 | 4.50645600 |
| H | 3.01513200 | 2.10758100 | 3.60602200 |
| O | -7.67914400 | -0.97457500 | -0.21303400 |
| O | 3.60439300 | -5.77901800 | -1.00207000 |
| O | 2.08577200 | 6.19765600 | -1.31761400 |
| C | -8.54176400 | 0.05381000 | 0.24084500 |
| H | -8.37651900 | 0.28249500 | 1.30254800 |
| H | -8.41962800 | 0.97398500 | -0.34653500 |
| H | -9.55722400 | -0.32501400 | 0.10888900 |
| C | 3.17036500 | 6.36091400 | -2.21631800 |
| H | 4.07597800 | 5.85579700 | -1.85429400 |
| H | 2.92555300 | 5.98431800 | -3.21846000 |
| H | 3.35525300 | 7.43538800 | -2.27101400 |
| C | 4.85192700 | -5.65005500 | -1.66332600 |
| H | 4.72980300 | -5.27412900 | -2.68802500 |
| H | 5.53324500 | -4.98492200 | -1.11581600 |
| H | 5.27890500 | -6.65415600 | -1.69696000 |

**Ar=4-CF3-Ph, R=Cy**

Zero-point correction= 0.507728 (Hartree/Particle)
Thermal correction to Energy= 0.543421
Thermal correction to Enthalpy= 0.544365
Thermal correction to Gibbs Free Energy= 0.432871
Sum of electronic and zero-point Energies= -2187.292029
Sum of electronic and thermal Energies= -2187.256336
Sum of electronic and thermal Enthalpies= -2187.255392
Sum of electronic and thermal Free Energies= -2187.366886
Single-point electronic energy (M06) = -2187.18016264

| | | | |
|---|---|---|---|
| C | 0.26911200 | -1.27192600 | 0.01687300 |
| C | 0.16313400 | 1.13445900 | 0.05527400 |
| C | -1.10267300 | -1.32477800 | -0.06892300 |
| C | -1.20676500 | 1.06708800 | -0.00327600 |
| C | -1.91611200 | -0.16650400 | 0.01290700 |
| H | -1.55548800 | -2.29239800 | -0.25262400 |
| H | -1.74496800 | 1.98792900 | -0.20262800 |
| N | 0.93533900 | -0.03942800 | 0.25062500 |
| C | 1.09842900 | -2.47185800 | -0.19994400 |
| C | 0.67302400 | -3.74277600 | 0.23650200 |
| C | 2.33225600 | -2.38556800 | -0.87538100 |
| C | 1.43494600 | -4.87811700 | -0.01112600 |
| H | -0.25105800 | -3.83450200 | 0.79908100 |
| C | 3.09657100 | -3.52027800 | -1.12268300 |
| H | 2.67663100 | -1.41759700 | -1.22467000 |
| C | 2.65194000 | -4.77388400 | -0.69291500 |
| H | 1.09662500 | -5.84631800 | 0.34397100 |
| H | 4.04013200 | -3.43443900 | -1.65144900 |
| C | 0.85557600 | 2.41043500 | -0.22689000 |
| C | 1.90444100 | 2.46543400 | -1.16526200 |
| C | 0.42979200 | 3.61204300 | 0.36540400 |
| C | 2.49960600 | 3.67466200 | -1.50024300 |
| H | 2.23251300 | 1.54893000 | -1.64489400 |
| C | 1.02844300 | 4.82561400 | 0.03571700 |
| H | -0.36948500 | 3.59034500 | 1.10057400 |
| C | 2.06531600 | 4.86202000 | -0.89835500 |
| H | 3.29213000 | 3.70415200 | -2.24157400 |
| H | 0.69088500 | 5.74384600 | 0.50429300 |
| C | -3.37876100 | -0.21718200 | -0.01173200 |
| C | -4.14727800 | 0.86353500 | 0.47732300 |

| | | | |
|---|---|---|---|
| C | -4.08396800 | -1.33652900 | -0.50757800 |
| C | -5.53543100 | 0.83124400 | 0.46646800 |
| H | -3.64692200 | 1.72726000 | 0.90390300 |
| C | -5.47210300 | -1.37184800 | -0.51841300 |
| H | -3.54133800 | -2.18230000 | -0.91737700 |
| C | -6.21026000 | -0.28814200 | -0.03125900 |
| H | -6.10001200 | 1.66921000 | 0.86279000 |
| H | -5.98802000 | -2.24320900 | -0.90860900 |
| C | 1.90099000 | -0.07229200 | 1.41614900 |
| C | 3.22230400 | 0.68559700 | 1.22103600 |
| C | 1.21168100 | 0.34587500 | 2.72844400 |
| H | 2.16245000 | -1.12977400 | 1.50890000 |
| C | 4.15483300 | 0.42520600 | 2.41879000 |
| H | 3.04234400 | 1.76187300 | 1.14071000 |
| H | 3.70198500 | 0.36815300 | 0.28760200 |
| C | 2.14301200 | 0.11523500 | 3.93046700 |
| H | 0.93855400 | 1.40817800 | 2.67460100 |
| H | 0.27969300 | -0.21919500 | 2.85098200 |
| C | 3.49190700 | 0.82522100 | 3.74580900 |
| H | 5.09214100 | 0.97710100 | 2.27877100 |
| H | 4.42233700 | -0.64124200 | 2.45065700 |
| H | 1.65205500 | 0.45720100 | 4.84996400 |
| H | 2.31469300 | -0.96428000 | 4.05235900 |
| H | 4.15838600 | 0.59797500 | 4.58692700 |
| H | 3.33354800 | 1.91348000 | 3.75568900 |
| C | 3.44420900 | -6.01247600 | -1.00354500 |
| C | -7.70967800 | -0.29983800 | -0.09621300 |
| C | 2.75750000 | 6.15493100 | -1.22860900 |
| F | 3.04721800 | 6.24267800 | -2.54690100 |
| F | 2.00856500 | 7.23108700 | -0.90394900 |
| F | 3.93298000 | 6.27716500 | -0.56569100 |
| F | 4.75605600 | -5.74239800 | -1.18538100 |
| F | 3.00752200 | -6.61731400 | -2.13407000 |
| F | 3.35075800 | -6.92912900 | -0.01312900 |
| F | -8.17158500 | 0.24850500 | -1.24691900 |
| F | -8.26445700 | 0.40499800 | 0.91696800 |
| F | -8.20852000 | -1.55581300 | -0.03773100 |

**Ar=4-F-Ph, R=Cy**

Zero-point correction= 0.468842 (Hartree/Particle)
Thermal correction to Energy= 0.496047
Thermal correction to Enthalpy= 0.496992
Thermal correction to Gibbs Free Energy= 0.408862
Sum of electronic and zero-point Energies= -1473.915608
Sum of electronic and thermal Energies= -1473.888403
Sum of electronic and thermal Enthalpies= -1473.887458
Sum of electronic and thermal Free Energies= -1473.975588
Single-point electronic energy (M06) = -1473.79497939

| | | | |
|---|---|---|---|
| C | 0.02327200 | 1.30167000 | -0.22879100 |
| C | -0.06298800 | -1.10920100 | -0.24624700 |
| C | 1.39598400 | 1.24611400 | -0.19131000 |
| C | 1.30798500 | -1.14663000 | -0.18476500 |
| C | 2.10839400 | 0.02468700 | -0.07180300 |
| H | 1.93599100 | 2.17925400 | -0.30887600 |
| H | 1.78947900 | -2.10304800 | -0.36274600 |
| N | -0.75832700 | 0.12074700 | -0.09066900 |
| C | -0.68992100 | 2.57060000 | -0.47592400 |
| C | -0.22640400 | 3.78559900 | 0.06632000 |
| C | -1.84058700 | 2.60885200 | -1.28902000 |
| C | -0.86727400 | 4.99157900 | -0.20472300 |
| H | 0.63550800 | 3.78069000 | 0.72682300 |
| C | -2.49436600 | 3.80662300 | -1.56375500 |
| H | -2.20815000 | 1.68575400 | -1.72545400 |
| C | -1.99524300 | 4.98441900 | -1.01777700 |
| H | -0.51562400 | 5.92781800 | 0.21645600 |
| H | -3.37355600 | 3.84066900 | -2.19913700 |
| C | -0.82636500 | -2.32568300 | -0.60312600 |
| C | -1.79734300 | -2.29808800 | -1.62238500 |
| C | -0.54211100 | -3.56121800 | 0.00661800 |
| C | -2.46023100 | -3.45521600 | -2.02043500 |
| H | -2.01937700 | -1.35643300 | -2.11431000 |
| C | -1.19671300 | -4.72897900 | -0.38191500 |
| H | 0.19360200 | -3.60259600 | 0.80466900 |
| C | -2.14892300 | -4.65697700 | -1.39136500 |
| H | -3.20150800 | -3.44180900 | -2.81297200 |
| H | -0.98620700 | -5.68279000 | 0.09080700 |
| C | 3.56869600 | -0.04164500 | 0.02652000 |
| C | 4.20725900 | -1.18297500 | 0.56192700 |
| C | 4.39979700 | 1.01845600 | -0.40010200 |
| C | 5.59237100 | -1.26944000 | 0.66318000 |
| H | 3.60623000 | -2.00720500 | 0.93337500 |
| C | 5.78550900 | 0.94790500 | -0.30039600 |
| H | 3.96049300 | 1.90435700 | -0.84733100 |
| C | 6.36631600 | -0.19888700 | 0.23033900 |
| H | 6.07571300 | -2.14590200 | 1.08287200 |
| H | 6.41881800 | 1.76148600 | -0.63949900 |
| C | -1.82853000 | 0.20740600 | 0.97327800 |
| C | -3.20497800 | -0.35203500 | 0.58159900 |
| C | -1.35459000 | -0.37871200 | 2.31639300 |
| H | -1.96346600 | 1.28250800 | 1.12105900 |
| C | -4.23160100 | -0.04867400 | 1.68777300 |
| H | -3.15114800 | -1.43469000 | 0.43308100 |
| H | -3.52907300 | 0.08764600 | -0.36920200 |
| C | -2.38552400 | -0.10305600 | 3.42460300 |
| H | -1.20940900 | -1.46201800 | 2.21358500 |
| H | -0.38145100 | 0.05194800 | 2.58173300 |
| C | -3.78153300 | -0.61692200 | 3.04184700 |
| H | -5.20824600 | -0.46150000 | 1.40652600 |
| H | -4.36631700 | 1.03958800 | 1.77532800 |
| H | -2.05223200 | -0.56255500 | 4.36361300 |
| H | -2.43666500 | 0.98003800 | 3.60941800 |
| H | -4.50763600 | -0.35959500 | 3.82317100 |
| H | -3.75984500 | -1.71494500 | 2.98249900 |
| F | -2.79209500 | -5.78146700 | -1.77038400 |
| F | 7.71203500 | -0.27304900 | 0.32854600 |
| F | -2.62658200 | 6.14903500 | -1.27706800 |

**Ar=3,5-diF-Ph, R=Cy**

Zero-point correction= 0.443792 (Hartree/Particle)
Thermal correction to Energy= 0.473706
Thermal correction to Enthalpy= 0.474650
Thermal correction to Gibbs Free Energy= 0.379861
Sum of electronic and zero-point Energies= -1771.640088
Sum of electronic and thermal Energies= -1771.610174
Sum of electronic and thermal Enthalpies= -1771.609229
Sum of electronic and thermal Free Energies= -1771.704019
Single-point electronic energy (M06) = -1771.51744378

| | | | |
|---|---|---|---|
| C | -0.02796300 | 1.29604800 | -0.14144100 |
| C | -0.15685800 | -1.10716700 | -0.19969000 |
| C | 1.34439500 | 1.21860300 | -0.15897500 |
| C | 1.21421900 | -1.17212100 | -0.19074000 |
| C | 2.03749500 | -0.01642800 | -0.09025400 |
| H | 1.89484900 | 2.14469400 | -0.27821300 |
| H | 1.66986500 | -2.13459100 | -0.39838800 |
| N | -0.82294600 | 0.12852000 | 0.00160500 |
| C | -0.72343300 | 2.58241300 | -0.34337100 |
| C | -0.20224000 | 3.77382700 | 0.19628300 |
| C | -1.90565200 | 2.64249600 | -1.10650000 |
| C | -0.85203000 | 4.97457500 | -0.05168800 |
| H | 0.68110800 | 3.77103400 | 0.82435400 |
| C | -2.51638300 | 3.86968400 | -1.31949800 |
| H | -2.32810900 | 1.75018700 | -1.55234400 |
| C | -2.01702900 | 5.06221700 | -0.80625000 |
| C | -0.94928700 | -2.30475200 | -0.55914500 |
| C | -1.94293700 | -2.22962600 | -1.55192500 |
| C | -0.65965700 | -3.54981300 | 0.02583300 |
| C | -2.61173400 | -3.38454400 | -1.92990100 |
| H | -2.17879800 | -1.28975600 | -2.03650100 |
| C | -1.35947000 | -4.67546500 | -0.39021400 |
| H | 0.08729100 | -3.64457600 | 0.80591900 |
| C | -2.34694900 | -4.62967900 | -1.36714000 |
| C | 3.49812000 | -0.10806200 | -0.04790100 |

| | | | |
|---|---|---|---|
| C | 4.12784800 | -1.28906700 | 0.40338900 |
| C | 4.32061500 | 0.96857500 | -0.44643300 |
| C | 5.51135300 | -1.36340800 | 0.43960600 |
| H | 3.55533200 | -2.13698000 | 0.76002900 |
| C | 5.69907200 | 0.84048300 | -0.38778000 |
| H | 3.90907100 | 1.89197400 | -0.83543900 |
| C | 6.33818800 | -0.31478900 | 0.05108500 |
| C | -1.86739200 | 0.21405900 | 1.09417600 |
| C | -3.25965800 | -0.32594900 | 0.73453800 |
| C | -1.36094800 | -0.39348500 | 2.41561600 |
| H | -1.98546200 | 1.28865200 | 1.25736600 |
| C | -4.24980600 | -0.01844900 | 1.87241600 |
| H | -3.22291500 | -1.40818200 | 0.57803200 |
| H | -3.60599400 | 0.12366900 | -0.20333200 |
| C | -2.35633600 | -0.11713800 | 3.55590400 |
| H | -1.23238500 | -1.47724800 | 2.29667400 |
| H | -0.37543500 | 0.02239400 | 2.65798300 |
| C | -3.77017200 | -0.60654800 | 3.20762800 |
| H | -5.23928100 | -0.41455600 | 1.61394200 |
| H | -4.36649100 | 1.07069900 | 1.97302300 |
| H | -2.00195700 | -0.59279600 | 4.47873900 |
| H | -2.38591500 | 0.96419700 | 3.75476400 |
| H | -4.46956600 | -0.34571300 | 4.01156900 |
| H | -3.76733800 | -1.70412400 | 3.13796300 |
| H | -2.51249300 | 6.00937700 | -0.98077400 |
| H | 7.41761300 | -0.39246700 | 0.08878500 |
| H | -2.88447600 | -5.51832500 | -1.67482800 |
| F | -3.63923800 | 3.91324700 | -2.06349900 |
| F | -0.34435700 | 6.10511000 | 0.47695200 |
| F | 6.46081300 | 1.88033700 | -0.78597800 |
| F | 6.08530600 | -2.50026600 | 0.88463500 |
| F | -1.07911600 | -5.86076700 | 0.18536500 |
| F | -3.55342200 | -3.30390100 | -2.89040300 |

**Ar=3,5-diMe-Ph, R=Cy**

Zero-point correction= 0.658547 (Hartree/Particle)
Thermal correction to Energy= 0.694725
Thermal correction to Enthalpy= 0.695669
Thermal correction to Gibbs Free Energy= 0.583914
Sum of electronic and zero-point Energies= -1411.934138
Sum of electronic and thermal Energies= -1411.897959
Sum of electronic and thermal Enthalpies= -1411.897015
Sum of electronic and thermal Free Energies= -1412.008770
Single-point electronic energy (M06) = -1411.84106891

| | | | |
|---|---|---|---|
| C | -0.02737100 | 1.30199800 | -0.14146300 |
| C | -0.16331500 | -1.10654200 | -0.21378300 |
| C | 1.34442000 | 1.21802800 | -0.17276200 |
| C | 1.20796100 | -1.17134800 | -0.21913100 |
| C | 2.03753400 | -0.01896600 | -0.11901800 |
| H | 1.89622100 | 2.14383800 | -0.29000100 |
| H | 1.65943800 | -2.13342700 | -0.43836500 |
| N | -0.82416300 | 0.13241900 | 0.00230200 |
| C | -0.72349700 | 2.59241500 | -0.31944100 |
| C | -0.20619300 | 3.77653300 | 0.23507600 |
| C | -1.90927900 | 2.67367600 | -1.07434800 |
| C | -0.82916500 | 5.01072800 | 0.03130300 |
| H | 0.68590900 | 3.72662400 | 0.85420700 |
| C | -2.55636600 | 3.89223600 | -1.28518700 |
| H | -2.31194200 | 1.76736300 | -1.51764600 |
| C | -2.00420000 | 5.05360800 | -0.72802600 |
| C | -0.96488700 | -2.30203400 | -0.56132200 |
| C | -1.97240400 | -2.23278000 | -1.54134100 |
| C | -0.68130500 | -3.54756800 | 0.01905400 |
| C | -2.67986100 | -3.36808500 | -1.93602400 |
| H | -2.18843500 | -1.27445700 | -2.00537200 |
| C | -1.37392900 | -4.70380600 | -0.35991900 |
| H | 0.08509400 | -3.60951300 | 0.78816700 |
| C | -2.37076000 | -4.59738700 | -1.33386000 |
| C | 3.49930300 | -0.11544800 | -0.09018900 |
| C | 4.13455800 | -1.28681700 | 0.37397600 |
| C | 4.32738000 | 0.94603600 | -0.51343700 |
| C | 5.52424600 | -1.40776200 | 0.41312700 |
| H | 3.52904900 | -2.11049400 | 0.74239400 |
| C | 5.71870000 | 0.85404300 | -0.47869200 |
| H | 3.87975200 | 1.85388800 | -0.90767100 |
| C | 6.30842400 | -0.32911700 | -0.01384100 |
| C | -1.84769800 | 0.21299500 | 1.10890200 |
| C | -3.24820900 | -0.31789400 | 0.76540100 |
| C | -1.32743900 | -0.40918000 | 2.41867200 |
| H | -1.96028100 | 1.28643700 | 1.28423500 |
| C | -4.22104800 | -0.01919000 | 1.92009200 |
| H | -3.21746200 | -1.39793300 | 0.59325200 |
| H | -3.60390700 | 0.14589500 | -0.16207600 |
| C | -2.30505200 | -0.14114400 | 3.57574700 |
| H | -1.20388600 | -1.49187500 | 2.28661700 |
| H | -0.33703800 | 0.00092200 | 2.65056900 |
| C | -3.72528800 | -0.62293400 | 3.24254600 |
| H | -5.21692600 | -0.40819200 | 1.67340600 |
| H | -4.33095400 | 1.06948300 | 2.03514400 |
| H | -1.94068500 | -0.62623300 | 4.49024400 |
| H | -2.32977900 | 0.93854300 | 3.78501500 |
| H | -4.41329600 | -0.36961800 | 4.05922100 |
| H | -3.72586100 | -1.71972800 | 3.15997100 |
| H | -2.50248100 | 6.00895100 | -0.88489100 |
| H | 7.39389600 | -0.41040000 | 0.01684200 |
| H | -2.92033000 | -5.48875500 | -1.63227100 |
| C | -1.03404500 | -6.04020300 | 0.26003800 |
| H | -0.18428300 | -6.51144800 | -0.25192800 |
| H | -0.75668800 | -5.93471100 | 1.31468000 |
| H | -1.87705000 | -6.73647300 | 0.19989000 |
| C | -3.76523400 | -3.28204200 | -2.98520100 |
| H | -3.77017200 | -2.30366900 | -3.47590900 |
| H | -3.63563200 | -4.04653400 | -3.76051800 |
| H | -4.75898600 | -3.43692500 | -2.54481000 |
| C | 6.17589400 | -2.68264300 | 0.90016200 |
| H | 6.59697100 | -3.25920200 | 0.06578500 |
| H | 6.99942000 | -2.47350500 | 1.59303100 |
| H | 5.45760900 | -3.32812400 | 1.41599700 |
| C | 6.58206000 | 2.01065700 | -0.93047000 |
| H | 5.98456800 | 2.79506300 | -1.40604500 |
| H | 7.11360400 | 2.46614900 | -0.08463400 |
| H | 7.34372700 | 1.68622600 | -1.64973900 |
| C | -0.23806100 | 6.27688600 | 0.60881900 |
| H | 0.37275600 | 6.06744900 | 1.49323800 |
| H | 0.40827900 | 6.78251800 | -0.12118800 |
| H | -1.01859300 | 6.98952800 | 0.89711700 |
| C | -3.83615900 | 3.96126200 | -2.08767400 |
| H | -4.00396900 | 3.03929300 | -2.65346300 |
| H | -4.70734100 | 4.11169900 | -1.43632600 |
| H | -3.81945500 | 4.79514100 | -2.79900500 |

**Ar=Ph, R=iPr**

Zero-point correction= 0.427019 (Hartree/Particle)
Thermal correction to Energy= 0.449928
Thermal correction to Enthalpy= 0.450872
Thermal correction to Gibbs Free Energy= 0.372792
Sum of electronic and zero-point Energies= -1059.521583
Sum of electronic and thermal Energies= -1059.498674
Sum of electronic and thermal Enthalpies= -1059.497730
Sum of electronic and thermal Free Energies= -1059.575810
Single-point electronic energy (M06) = -1059.39458891

| | | | |
|---|---|---|---|
| C | -2.01460900 | 0.14985800 | 1.40712000 |
| H | -2.19033200 | 1.21943100 | 1.53557000 |
| C | -0.32162600 | 1.27370700 | 0.01512700 |
| C | -0.37462100 | -1.13809800 | 0.00394300 |
| C | 1.04907400 | 1.23642900 | -0.08712800 |
| C | 0.99557600 | -1.15735100 | -0.07236900 |
| C | 1.78685600 | 0.02560000 | -0.04266100 |
| H | 1.56186500 | 2.17662700 | -0.25602600 |
| H | 1.46920200 | -2.10819100 | -0.29428000 |
| N | -1.06747800 | 0.08163400 | 0.22775300 |

| | | | |
|---|---|---|---|
| C | -1.07412700 | 2.53195500 | -0.15802100 |
| C | -0.56572700 | 3.75768400 | 0.31528000 |
| C | -2.31236200 | 2.54713900 | -0.83109900 |
| C | -1.25683100 | 4.94882700 | 0.10691800 |
| H | 0.36784000 | 3.76818400 | 0.87067300 |
| C | -3.00294900 | 3.73921500 | -1.03426400 |
| H | -2.71446900 | 1.61405900 | -1.21378400 |
| C | -2.47983200 | 4.94792400 | -0.56831400 |
| H | -0.84474600 | 5.88049900 | 0.48599100 |
| H | -3.95072000 | 3.72556900 | -1.56654500 |
| C | -1.15401300 | -2.36619200 | -0.27085300 |
| C | -2.21803000 | -2.35367800 | -1.19200700 |
| C | -0.79929600 | -3.59287500 | 0.31866200 |
| C | -2.89875400 | -3.52535900 | -1.51206900 |
| H | -2.49231500 | -1.41620700 | -1.66620000 |
| C | -1.48337400 | -4.76520400 | -0.00147700 |
| H | 0.01094300 | -3.61828600 | 1.04246600 |
| C | -2.53643200 | -4.73762700 | -0.91737200 |
| H | -3.71019000 | -3.49521100 | -2.23479500 |
| H | -1.19676200 | -5.70081700 | 0.47175400 |
| C | -3.38314600 | -0.49798700 | 1.17892100 |
| H | -3.33280600 | -1.58808200 | 1.14482200 |
| H | -4.04287800 | -0.21708400 | 2.00863900 |
| H | -3.84095700 | -0.14336100 | 0.25059400 |
| C | -1.33910400 | -0.36890600 | 2.68445500 |
| H | -1.97735100 | -0.16315500 | 3.55149900 |
| H | -1.17259200 | -1.45023300 | 2.63888300 |
| H | -0.37401600 | 0.12274600 | 2.84541200 |
| C | 3.25063800 | -0.01980400 | -0.09148200 |
| C | 3.95422700 | -1.15804500 | 0.36232000 |
| C | 4.01956900 | 1.05858800 | -0.58305600 |
| C | 5.34417900 | -1.21589000 | 0.32242300 |
| H | 3.40223600 | -1.99542600 | 0.77922900 |
| C | 5.40930000 | 0.99952300 | -0.61902500 |
| H | 3.52350900 | 1.94308800 | -0.97106100 |
| C | 6.08479800 | -0.13764600 | -0.16783800 |
| H | 5.85285200 | -2.10522500 | 0.68633900 |
| H | 5.96932000 | 1.84442500 | -1.01224500 |
| H | 7.16994900 | -0.18190700 | -0.19726600 |
| H | -3.07067800 | -5.65061100 | -1.16571300 |
| H | -3.02084900 | 5.87701200 | -0.72503500 |

**Ar=4-Me-Ph, R=iPr**

Zero-point correction= 0.509460 (Hartree/Particle)
Thermal correction to Energy= 0.538079
Thermal correction to Enthalpy= 0.539023
Thermal correction to Gibbs Free Energy= 0.446616
Sum of electronic and zero-point Energies= -1177.393364
Sum of electronic and thermal Energies= -1177.364745
Sum of electronic and thermal Enthalpies= -1177.363801
Sum of electronic and thermal Free Energies= -1177.456208
Single-point electronic energy (M06) = -1177.27900367

| | | | |
|---|---|---|---|
| C | 2.00958400 | -0.03233700 | 1.55021100 |
| H | 2.24392700 | -1.09084200 | 1.67760300 |
| C | 0.44295700 | -1.24715000 | 0.09009500 |
| C | 0.33240100 | 1.16357900 | 0.11101800 |
| C | -0.92440700 | -1.30070600 | -0.04356800 |
| C | -1.03377100 | 1.09109600 | 0.00091400 |
| C | -1.74376500 | -0.14303000 | 0.00046300 |
| H | -1.36882400 | -2.27018100 | -0.23927700 |
| H | -1.56531100 | 2.01031700 | -0.22323400 |
| N | 1.10019000 | -0.01018200 | 0.34038500 |
| C | 1.28479100 | -2.44659000 | -0.08153800 |
| C | 0.85133500 | -3.71620000 | 0.34583000 |
| C | 2.54184600 | -2.36959200 | -0.71280700 |
| C | 1.62878900 | -4.85076100 | 0.13355400 |
| H | -0.09788800 | -3.80940400 | 0.86607600 |
| C | 3.31425400 | -3.50858700 | -0.91773200 |
| H | 2.89482400 | -1.40600800 | -1.06759600 |
| C | 2.87736400 | -4.77309700 | -0.49869100 |
| H | 1.26358800 | -5.81635900 | 0.47725300 |
| H | 4.27359000 | -3.41600400 | -1.42301600 |
| C | 1.03598800 | 2.44283700 | -0.12643600 |
| C | 2.13284900 | 2.51597900 | -1.00520800 |
| C | 0.58058100 | 3.64103400 | 0.44939300 |
| C | 2.74052400 | 3.73340900 | -1.29227400 |
| H | 2.49056900 | 1.60637900 | -1.47830100 |
| C | 1.19565300 | 4.85755700 | 0.15826700 |
| H | -0.25876300 | 3.61378200 | 1.13934700 |
| C | 2.28848900 | 4.92957500 | -0.71383200 |
| H | 3.57696800 | 3.76005300 | -1.98790100 |
| H | 0.82217200 | 5.76750200 | 0.62322700 |
| C | 3.34501200 | 0.69613200 | 1.37230300 |
| H | 3.23302900 | 1.78198900 | 1.34589100 |
| H | 3.99372600 | 0.44519000 | 2.22026100 |
| H | 3.85168900 | 0.37815300 | 0.45611300 |
| C | 1.26384400 | 0.43456700 | 2.80826700 |
| H | 1.88584700 | 0.26126600 | 3.69407200 |
| H | 1.03299100 | 1.50397100 | 2.76333400 |
| H | 0.32604800 | -0.11631300 | 2.93469000 |
| C | -3.20519100 | -0.19560400 | -0.07710600 |
| C | -3.99678300 | 0.88812000 | 0.36296400 |
| C | -3.89631500 | -1.32074500 | -0.57743700 |
| C | -5.38537700 | 0.84852700 | 0.29963900 |
| H | -3.51575400 | 1.76152000 | 0.79376000 |
| C | -5.28512000 | -1.35339200 | -0.63513800 |
| H | -3.34057000 | -2.17569000 | -0.95099800 |
| C | -6.06366400 | -0.27040000 | -0.20274800 |
| H | -5.95701700 | 1.70160200 | 0.66021000 |
| H | -5.77771400 | -2.23853600 | -1.03307000 |
| C | -7.57047000 | -0.29889900 | -0.29757100 |
| H | -7.92114900 | 0.09732200 | -1.26080600 |
| H | -7.95928100 | -1.31928100 | -0.20803800 |
| H | -8.03355700 | 0.30846800 | 0.48804000 |
| C | 2.97508400 | 6.24285600 | -1.00587100 |
| H | 3.29515000 | 6.30392700 | -2.05218000 |
| H | 2.31576400 | 7.09357600 | -0.80440000 |
| H | 3.87312200 | 6.37197300 | -0.38643300 |
| C | 3.73467700 | -6.00116000 | -0.69278000 |
| H | 4.41605000 | -6.15311400 | 0.15570200 |
| H | 3.12458900 | -6.90636000 | -0.78326900 |
| H | 4.35390600 | -5.91972000 | -1.59283600 |

**Ar=4-MeO-Ph, R=iPr**

Zero-point correction= 0.525211 (Hartree/Particle)
Thermal correction to Energy= 0.555999
Thermal correction to Enthalpy= 0.556943
Thermal correction to Gibbs Free Energy= 0.460750
Sum of electronic and zero-point Energies= -1402.990634
Sum of electronic and thermal Energies= -1402.959846
Sum of electronic and thermal Enthalpies= -1402.958902
Sum of electronic and thermal Free Energies= -1403.055095
Single-point electronic energy (M06) = -1402.87863584

| | | | |
|---|---|---|---|
| C | 1.85909300 | 0.16421600 | 1.77486700 |
| H | 2.25456300 | -0.84717900 | 1.88680200 |
| C | 0.58673100 | -1.21995000 | 0.19099400 |
| C | 0.13949500 | 1.15218600 | 0.23449100 |
| C | -0.75232500 | -1.46074900 | -0.00637700 |
| C | -1.19643800 | 0.89187800 | 0.05806500 |
| C | -1.72751700 | -0.42910800 | 0.01601500 |
| H | -1.04679200 | -2.47780100 | -0.24093800 |
| H | -1.84058000 | 1.73013100 | -0.18845500 |
| N | 1.05266300 | 0.09209000 | 0.49554800 |
| C | 1.59822800 | -2.28240800 | 0.03955100 |
| C | 1.32643400 | -3.61933400 | 0.40308900 |
| C | 2.86535600 | -2.01060300 | -0.50407900 |
| C | 2.25965300 | -4.62616900 | 0.21149000 |
| H | 0.37327500 | -3.86412500 | 0.86293900 |
| C | 3.81552400 | -3.01346400 | -0.69787700 |
| H | 3.10138200 | -0.99370700 | -0.80237400 |
| C | 3.51538200 | -4.33386100 | -0.34304800 |
| H | 2.04599700 | -5.65119200 | 0.49861800 |

| | | | |
|---|---|---|---|
| H | 4.77519700 | -2.75626300 | -1.13215000 |
| C | 0.67204300 | 2.51771400 | 0.04389500 |
| C | 1.80633700 | 2.75348100 | -0.74836500 |
| C | 0.01361400 | 3.64076400 | 0.58446200 |
| C | 2.27268100 | 4.04365600 | -0.99908700 |
| H | 2.32419200 | 1.90736500 | -1.18966300 |
| C | 0.46600700 | 4.93055500 | 0.34408200 |
| H | -0.85880500 | 3.49169500 | 1.21496500 |
| C | 1.60148000 | 5.14436900 | -0.45082400 |
| H | 3.14702600 | 4.17885100 | -1.62608200 |
| H | -0.03885500 | 5.79219800 | 0.76999900 |
| C | 3.06503700 | 1.10711800 | 1.72940800 |
| H | 2.77630100 | 2.16030600 | 1.72815500 |
| H | 3.68055600 | 0.92805200 | 2.61930600 |
| H | 3.68460700 | 0.91732900 | 0.84760300 |
| C | 0.95539600 | 0.45000900 | 2.98266200 |
| H | 1.52859400 | 0.34292100 | 3.91099600 |
| H | 0.55509300 | 1.46882200 | 2.94978500 |
| H | 0.11395000 | -0.24974800 | 3.01723800 |
| C | -3.16263800 | -0.68297900 | -0.12494800 |
| C | -4.11613400 | 0.27197400 | 0.28054300 |
| C | -3.67055500 | -1.88914500 | -0.66431400 |
| C | -5.48831000 | 0.05584200 | 0.15659400 |
| H | -3.78210000 | 1.20092000 | 0.73320100 |
| C | -5.03082600 | -2.11872500 | -0.78955500 |
| H | -2.98614100 | -2.65324200 | -1.01963300 |
| C | -5.95786600 | -1.14757300 | -0.38090500 |
| H | -6.17589700 | 0.82408700 | 0.49267300 |
| H | -5.40502500 | -3.04509600 | -1.21498700 |
| O | -7.27610400 | -1.47159900 | -0.54713500 |
| O | 1.96948900 | 6.44812000 | -0.62472900 |
| O | 4.36440900 | -5.39416600 | -0.48588300 |
| C | -8.25034300 | -0.51791800 | -0.16090900 |
| H | -8.14854000 | 0.41742900 | -0.72784900 |
| H | -9.21893000 | -0.97001100 | -0.38342000 |
| H | -8.19440200 | -0.29323700 | 0.91295500 |
| C | 5.64728100 | -5.15474800 | -1.04020900 |
| H | 6.14954200 | -6.12368500 | -1.06376500 |
| H | 5.57873300 | -4.75757500 | -2.06187900 |
| H | 6.23158700 | -4.45896800 | -0.42303400 |
| C | 3.10936100 | 6.72197000 | -1.42249300 |
| H | 3.21945700 | 7.80803400 | -1.42530300 |
| H | 4.01636500 | 6.26713700 | -1.00204700 |
| H | 2.97558300 | 6.36910500 | -2.45382900 |

**Ar=4-CF3-Ph, R=iPr**

Zero-point correction= 0.441261 (Hartree/Particle)
Thermal correction to Energy= 0.475226
Thermal correction to Enthalpy= 0.476171
Thermal correction to Gibbs Free Energy= 0.368726
Sum of electronic and zero-point Energies= -2070.621809
Sum of electronic and thermal Energies= -2070.587844
Sum of electronic and thermal Enthalpies= -2070.586900
Sum of electronic and thermal Free Energies= -2070.694345
Single-point electronic energy (M06) = -2070.50289602

| | | | |
|---|---|---|---|
| C | 2.08077800 | 0.22704300 | 1.76458900 |
| H | 2.43380500 | -0.79838700 | 1.88719400 |
| C | 0.68480900 | -1.16195100 | 0.27847800 |
| C | 0.24852500 | 1.20645400 | 0.34075500 |
| C | -0.65863400 | -1.39930700 | 0.10581400 |
| C | -1.09291300 | 0.95365100 | 0.19253700 |
| C | -1.62709400 | -0.36413700 | 0.14306200 |
| H | -0.96053100 | -2.41697300 | -0.11351300 |
| H | -1.73897700 | 1.79848700 | -0.02183000 |
| N | 1.16302000 | 0.14480200 | 0.55941800 |
| C | 1.67945500 | -2.23716600 | 0.10277400 |
| C | 1.41183300 | -3.55466000 | 0.52302500 |
| C | 2.91417400 | -1.98303700 | -0.52839000 |
| C | 2.32910400 | -4.57721300 | 0.30682700 |
| H | 0.48366500 | -3.77276700 | 1.04254500 |
| C | 3.83218700 | -3.00332600 | -0.74442300 |
| H | 3.13329700 | -0.97832700 | -0.87491700 |
| C | 3.54438900 | -4.30770100 | -0.32875400 |
| H | 2.10473600 | -5.58606400 | 0.63695600 |
| H | 4.76828700 | -2.79323800 | -1.25206600 |
| C | 0.76694200 | 2.57778500 | 0.14566200 |
| C | 1.85881000 | 2.82420900 | -0.70792800 |
| C | 0.13097600 | 3.67972800 | 0.74560700 |
| C | 2.29439800 | 4.12042900 | -0.95517600 |
| H | 2.35425900 | 1.98694600 | -1.18859000 |
| C | 0.56567400 | 4.97929300 | 0.50115000 |
| H | -0.70033900 | 3.51021100 | 1.42373300 |
| C | 1.65060700 | 5.20512100 | -0.34915800 |
| H | 3.13459400 | 4.29450100 | -1.61978800 |
| H | 0.07327800 | 5.81739800 | 0.98308900 |
| C | 3.32301700 | 1.10282800 | 1.57961900 |
| H | 3.08921800 | 2.16923500 | 1.56662400 |
| H | 4.00335700 | 0.92046100 | 2.41966000 |
| H | 3.85663500 | 0.85274600 | 0.65763100 |
| C | 1.29300100 | 0.60208600 | 3.02708200 |
| H | 1.93606400 | 0.49349600 | 3.90755700 |
| H | 0.94607900 | 1.63990900 | 2.99189700 |
| H | 0.42335700 | -0.05044000 | 3.15617400 |
| C | -3.06375800 | -0.61400900 | 0.01715400 |
| C | -4.00668200 | 0.34454800 | 0.45272400 |
| C | -3.57158600 | -1.81096600 | -0.53615100 |
| C | -5.37293900 | 0.12239000 | 0.34168700 |
| H | -3.66263800 | 1.26631700 | 0.91115800 |
| C | -4.93720500 | -2.03663800 | -0.64601300 |
| H | -2.89034100 | -2.56399200 | -0.91856900 |
| C | -5.85035900 | -1.07138900 | -0.20861700 |
| H | -6.07398800 | 0.87618700 | 0.68560900 |
| H | -5.29904700 | -2.95833600 | -1.09018000 |
| C | 2.09282000 | 6.60826500 | -0.65916000 |
| C | 4.56672000 | -5.39404500 | -0.51119000 |
| C | -7.32586700 | -1.33863800 | -0.27143600 |
| F | 1.49345000 | 7.08867700 | -1.77432600 |
| F | 1.79673000 | 7.46404700 | 0.34426800 |
| F | 3.42621000 | 6.67789900 | -0.87368400 |
| F | 5.47026300 | -5.40886400 | 0.49863100 |
| F | 4.00077000 | -6.62053300 | -0.54807700 |
| F | 5.26825500 | -5.23385700 | -1.65625400 |
| F | -8.03879300 | -0.20021500 | -0.43276200 |
| F | -7.78373700 | -1.92442700 | 0.86267300 |
| F | -7.64681500 | -2.16704400 | -1.29148900 |

**Ar=4-F-Ph, R=iPr**

Zero-point correction= 0.402139 (Hartree/Particle)
Thermal correction to Energy= 0.427638
Thermal correction to Enthalpy= 0.428582
Thermal correction to Gibbs Free Energy= 0.344314
Sum of electronic and zero-point Energies= -1357.245686
Sum of electronic and thermal Energies= -1357.220186
Sum of electronic and thermal Enthalpies= -1357.219242
Sum of electronic and thermal Free Energies= -1357.303510
Single-point electronic energy (M06) = -1357.11799303

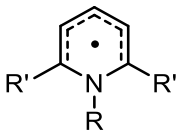
| | | | |
|---|---|---|---|
| C | 2.00993900 | -0.04636500 | 1.54649700 |
| H | 2.24362600 | -1.10552100 | 1.66954100 |
| C | 0.43297400 | -1.24951600 | 0.08602600 |
| C | 0.34344300 | 1.16103800 | 0.10319400 |
| C | -0.93472800 | -1.29210900 | -0.04571700 |
| C | -1.02330000 | 1.10094000 | -0.00497900 |
| C | -1.74344900 | -0.12707700 | -0.00162900 |
| H | -1.38831100 | -2.25788400 | -0.23958600 |
| H | -1.54751400 | 2.02383200 | -0.23214000 |
| N | 1.10238000 | -0.01845200 | 0.33375500 |
| C | 1.26485300 | -2.45676300 | -0.08505300 |
| C | 0.82129800 | -3.71919500 | 0.35667100 |
| C | 2.51905500 | -2.38701000 | -0.72488400 |
| C | 1.58149500 | -4.86734400 | 0.15171900 |
| H | -0.12287600 | -3.79833600 | 0.88712600 |
| C | 3.29203600 | -3.52601700 | -0.93120700 |

| | | | |
|---|---|---|---|
| H | 2.87574800 | -1.42608100 | -1.08152300 |
| C | 2.80952200 | -4.75375600 | -0.49078800 |
| H | 1.24419600 | -5.83955800 | 0.49612400 |
| H | 4.25256600 | -3.47662600 | -1.43398400 |
| C | 1.05895200 | 2.43347900 | -0.13895900 |
| C | 2.14924800 | 2.49039800 | -1.02789300 |
| C | 0.61948700 | 3.63406900 | 0.44772100 |
| C | 2.77802100 | 3.69599000 | -1.32369600 |
| H | 2.49204200 | 1.57583200 | -1.50122900 |
| C | 1.23879600 | 4.84961900 | 0.16101400 |
| H | -0.21090600 | 3.61107500 | 1.14765200 |
| C | 2.31156400 | 4.86111900 | -0.72204900 |
| H | 3.61145600 | 3.74777700 | -2.01686900 |
| H | 0.90854000 | 5.77734300 | 0.61682600 |
| C | 3.34545400 | 0.68271500 | 1.37313400 |
| H | 3.23433500 | 1.76889700 | 1.35553700 |
| H | 3.99417700 | 0.42614800 | 2.21908400 |
| H | 3.85303600 | 0.37164000 | 0.45494600 |
| C | 1.26190000 | 0.41500000 | 2.80485700 |
| H | 1.88230100 | 0.23802800 | 3.69083700 |
| H | 1.03144800 | 1.48471000 | 2.76461800 |
| H | 0.32385600 | -0.13620000 | 2.92780500 |
| C | -3.20608500 | -0.16698400 | -0.07836100 |
| C | -3.98447700 | 0.91804400 | 0.38413700 |
| C | -3.90163600 | -1.27814000 | -0.60577200 |
| C | -5.37442800 | 0.90338200 | 0.32168200 |
| H | -3.49276100 | 1.77806400 | 0.82817700 |
| C | -5.29086600 | -1.30851800 | -0.67022500 |
| H | -3.34927300 | -2.12462000 | -1.00132500 |
| C | -6.01195300 | -0.21384700 | -0.20539800 |
| H | -5.96640500 | 1.73671800 | 0.68646600 |
| H | -5.81909800 | -2.16077800 | -1.08566100 |
| F | 2.92042800 | 6.03264500 | -1.00201000 |
| F | -7.36158500 | -0.23803500 | -0.26586700 |
| F | 3.55565300 | -5.86174400 | -0.68422900 |

**Ar=3,5-diF-Ph, R=iPr**

Zero-point correction= 0.377262 (Hartree/Particle)
Thermal correction to Energy= 0.405408
Thermal correction to Enthalpy= 0.406352
Thermal correction to Gibbs Free Energy= 0.315813
Sum of electronic and zero-point Energies= -1654.969943
Sum of electronic and thermal Energies= -1654.941797
Sum of electronic and thermal Enthalpies= -1654.940853
Sum of electronic and thermal Free Energies= -1655.031392
Single-point electronic energy (M06) = -1654.84035734

| | | | |
|---|---|---|---|
| C | -2.00618800 | 0.05531600 | 1.64210300 |
| H | -2.22221600 | 1.11607000 | 1.78075800 |
| C | -0.43462700 | 1.24766000 | 0.16392400 |
| C | -0.39535700 | -1.15916100 | 0.13943700 |
| C | 0.92860300 | 1.26648800 | -0.01397300 |
| C | 0.96794900 | -1.12837400 | -0.01301400 |
| C | 1.71187900 | 0.08465700 | -0.01703400 |
| H | 1.39466300 | 2.22602200 | -0.20582300 |
| H | 1.46378700 | -2.05950200 | -0.26621300 |
| N | -1.12031500 | 0.02924200 | 0.41063200 |
| C | -1.24309000 | 2.47528000 | 0.03160100 |
| C | -0.74603700 | 3.71700700 | 0.47170700 |
| C | -2.51660400 | 2.42789800 | -0.56832400 |
| C | -1.50982500 | 4.86043300 | 0.28575600 |
| H | 0.20982700 | 3.79783000 | 0.97630000 |
| C | -3.23925600 | 3.60156600 | -0.72513800 |
| H | -2.92673200 | 1.49455800 | -0.93485700 |
| C | -2.76677900 | 4.84193500 | -0.30937200 |
| C | -1.14137500 | -2.41315800 | -0.11051400 |
| C | -2.24797900 | -2.41941500 | -0.97860600 |
| C | -0.70459100 | -3.62562300 | 0.45072000 |
| C | -2.88043000 | -3.62096500 | -1.26126900 |
| H | -2.59860400 | -1.50564400 | -1.44327700 |
| C | -1.37467700 | -4.80081600 | 0.13401800 |
| H | 0.13377300 | -3.65859100 | 1.13744300 |
| C | -2.47101800 | -4.83583000 | -0.71929300 |
| C | -3.35348100 | -0.65482100 | 1.48863300 |
| H | -3.25618400 | -1.74204100 | 1.46097300 |
| H | -3.97913700 | -0.39742600 | 2.35123400 |
| H | -3.87807500 | -0.33011200 | 0.58520300 |
| C | -1.23506800 | -0.43092300 | 2.87664500 |
| H | -1.83446200 | -0.25897800 | 3.77761500 |
| H | -1.01804700 | -1.50255200 | 2.81761700 |
| H | -0.28862900 | 0.10837600 | 2.98723900 |
| C | 3.17083700 | 0.09745500 | -0.14134100 |
| C | 3.93056900 | -1.03120900 | 0.23788900 |
| C | 3.86351000 | 1.22651900 | -0.63124800 |
| C | 5.31123000 | -1.00579200 | 0.11900800 |
| H | 3.46413900 | -1.91491400 | 0.65687200 |
| C | 5.24549800 | 1.19799400 | -0.72761100 |
| H | 3.34538100 | 2.11518400 | -0.97098700 |
| C | 6.01134900 | 0.09571000 | -0.36131300 |
| H | -3.34952600 | 5.74581300 | -0.43769700 |
| H | 7.09104200 | 0.09617800 | -0.44426100 |
| H | -2.98243700 | -5.76227800 | -0.95041100 |
| F | 5.88083400 | 2.28606400 | -1.20950700 |
| F | 6.01190200 | -2.09413000 | 0.49874000 |
| F | -3.93170100 | -3.61834300 | -2.10412300 |
| F | -0.95293300 | -5.95482700 | 0.68622100 |
| F | -4.44994300 | 3.54209300 | -1.31395100 |
| F | -1.02222600 | 6.04006900 | 0.71678800 |




**R'=H, R=iPr**

Zero-point correction= 0.182923 (Hartree/Particle)
Thermal correction to Energy= 0.192108
Thermal correction to Enthalpy= 0.193052
Thermal correction to Gibbs Free Energy= 0.148087
Sum of electronic and zero-point Energies= -366.595521
Sum of electronic and thermal Energies= -366.586337
Sum of electronic and thermal Enthalpies= -366.585393
Sum of electronic and thermal Free Energies= -366.630357
Single-point electronic energy (M06) = -366.58825

| | | | |
|---|---|---|---|
| C | -1.59835200 | -0.38767000 | -0.14831300 |
| H | -1.75745400 | -1.36327100 | -0.62318800 |
| C | 0.72702900 | -1.20190300 | -0.40710500 |
| C | 0.37806300 | 1.12300300 | 0.08432200 |
| C | 2.07081900 | -1.05071400 | -0.21593300 |
| C | 1.72107600 | 1.28656000 | 0.27968800 |
| C | 2.62811300 | 0.20689900 | 0.13321600 |
| H | 2.70668400 | -1.92248000 | -0.34438400 |
| H | 2.07957900 | 2.27654400 | 0.54891000 |
| N | -0.16055600 | -0.11673500 | -0.30648000 |
| C | -1.99750600 | -0.50344600 | 1.33232200 |
| H | -1.84047300 | 0.44859400 | 1.85222000 |
| H | -3.05473900 | -0.77568600 | 1.43085000 |
| H | -1.39455700 | -1.26649500 | 1.83567700 |
| C | -2.46026400 | 0.63317800 | -0.90262800 |
| H | -3.50819200 | 0.31454100 | -0.88706700 |
| H | -2.41674500 | 1.62790600 | -0.44563000 |
| H | -2.13901500 | 0.71937400 | -1.94545000 |
| H | 0.27194500 | -2.14606000 | -0.68429100 |
| H | -0.32885500 | 1.93650600 | 0.18017800 |
| H | 3.69184700 | 0.33222800 | 0.29412100 |

**R'=Me, R=iPr**

Zero-point correction= 0.239859 (Hartree/Particle)
Thermal correction to Energy= 0.251764
Thermal correction to Enthalpy= 0.252708
Thermal correction to Gibbs Free Energy= 0.202327
Sum of electronic and zero-point Energies= -445.164746
Sum of electronic and thermal Energies= -445.152840
Sum of electronic and thermal Enthalpies= -445.151896

Sum of electronic and thermal Free Energies= -445.202277
Single-point electronic energy (M06) = -445.17059

| | | | |
|---|---|---|---|
| C | 1.43998900 | -0.62912300 | 0.23471300 |
| H | 1.34043400 | -1.71271100 | 0.29173300 |
| C | -0.97600800 | -1.07608500 | -0.15596600 |
| C | -0.21253800 | 1.23652700 | -0.19650500 |
| C | -2.24545400 | -0.63873600 | 0.12401300 |
| C | -1.49268700 | 1.64020300 | 0.09474400 |
| C | -2.54098800 | 0.72652500 | 0.32639800 |
| H | -3.04160100 | -1.37861000 | 0.14763900 |
| H | -1.69490500 | 2.70848100 | 0.09356100 |
| N | 0.10654500 | -0.15257300 | -0.23014200 |
| C | 2.58409400 | -0.37914800 | -0.76251300 |
| H | 2.91497700 | 0.66104000 | -0.79071600 |
| H | 3.44852000 | -0.99002200 | -0.47609700 |
| H | 2.28183700 | -0.67087900 | -1.77369900 |
| C | 1.76584100 | -0.15117500 | 1.66005700 |
| H | 2.69130700 | -0.62234400 | 2.01191900 |
| H | 1.90152000 | 0.93301300 | 1.71495300 |
| H | 0.95881400 | -0.42449700 | 2.34788000 |
| H | -3.54314700 | 1.06128700 | 0.56712200 |
| C | 0.82702200 | 2.24126000 | -0.61567700 |
| H | 1.70093000 | 2.28676000 | 0.04565100 |
| H | 1.20159500 | 2.03723300 | -1.62790800 |
| H | 0.37800400 | 3.23862600 | -0.62241100 |
| C | -0.70619400 | -2.52345600 | -0.47718300 |
| H | -0.19383900 | -3.07259700 | 0.32600800 |
| H | -1.65514400 | -3.03774200 | -0.65446700 |
| H | -0.09358300 | -2.62978500 | -1.38266600 |

**R'=Ph, R=iPr**
Zero-point correction= 0.345810 (Hartree/Particle)
Thermal correction to Energy= 0.363879
Thermal correction to Enthalpy= 0.364824
Thermal correction to Gibbs Free Energy= 0.298704
Sum of electronic and zero-point Energies= -828.541184
Sum of electronic and thermal Energies= -828.523115
Sum of electronic and thermal Enthalpies= -828.522170
Sum of electronic and thermal Free Energies= -828.588290
Single-point electronic energy (M06) = -828.449

| | | | |
|---|---|---|---|
| C | -0.13036100 | -0.32338500 | 1.54212500 |
| H | -1.19677000 | -0.49882700 | 1.69747000 |
| C | -1.28224600 | 0.92515300 | -0.23789300 |
| C | 1.14630100 | 0.92677800 | -0.22509600 |
| C | -1.26984100 | 2.24930000 | -0.63149600 |
| C | 1.13591400 | 2.25255700 | -0.60571700 |
| C | -0.06826400 | 2.96865100 | -0.74280700 |
| H | -2.20467000 | 2.70600700 | -0.94186500 |
| H | 2.07613000 | 2.70892900 | -0.90172000 |
| N | -0.06818800 | 0.28857700 | 0.15798400 |
| C | -2.50536100 | 0.10731700 | -0.27391800 |
| C | -3.77186500 | 0.67115700 | -0.01382200 |
| C | -2.45164100 | -1.26492100 | -0.59584500 |
| C | -4.92992000 | -0.09727500 | -0.09320900 |
| H | -3.84119500 | 1.71589700 | 0.27558600 |
| C | -3.61168900 | -2.03132300 | -0.67040900 |
| H | -1.48778300 | -1.71522500 | -0.81180000 |
| C | -4.85923500 | -1.45383900 | -0.42153400 |
| H | -5.89253800 | 0.36247900 | 0.11599900 |
| H | -3.54210000 | -3.08407800 | -0.93282700 |
| H | -5.76366500 | -2.05328900 | -0.47740300 |
| C | 2.38195000 | 0.12488600 | -0.31822500 |
| C | 2.37567300 | -1.14721200 | -0.92308100 |
| C | 3.61513000 | 0.64127300 | 0.12358900 |
| C | 3.55487000 | -1.86992900 | -1.08084500 |
| H | 1.43534200 | -1.55263100 | -1.28391100 |
| C | 4.79470700 | -0.08444000 | -0.03500100 |
| H | 3.63924300 | 1.61315100 | 0.60933000 |
| C | 4.77185000 | -1.34416400 | -0.63688700 |
| H | 3.52666700 | -2.84503700 | -1.56070800 |
| H | 5.73333600 | 0.33248700 | 0.32112900 |
| H | 5.69081000 | -1.91112000 | -0.75803100 |
| C | 0.56662000 | -1.67908700 | 1.68913400 |
| H | 1.65523600 | -1.59945600 | 1.65640100 |
| H | 0.29008400 | -2.10757600 | 2.66002300 |
| H | 0.24761600 | -2.37842500 | 0.91050500 |
| C | 0.33941000 | 0.67860100 | 2.60655800 |
| H | 0.14243600 | 0.27751400 | 3.60754100 |
| H | 1.41439000 | 0.87144700 | 2.52666700 |
| H | -0.19052100 | 1.63167800 | 2.50866500 |
| H | -0.06674800 | 4.00545100 | -1.06067900 |

**R'=CF3, R=iPr**
Zero-point correction= 0.193948 (Hartree/Particle)
Thermal correction to Energy= 0.209657
Thermal correction to Enthalpy= 0.210601
Thermal correction to Gibbs Free Energy= 0.150548
Sum of electronic and zero-point Energies= -1040.649160
Sum of electronic and thermal Energies= -1040.633451
Sum of electronic and thermal Enthalpies= -1040.632507
Sum of electronic and thermal Free Energies= -1040.692559
Single-point electronic energy (M06) = -1040.6421

| | | | |
|---|---|---|---|
| C | -0.08352900 | -1.48494100 | 0.65751500 |
| H | -1.14264400 | -1.70937500 | 0.76162400 |
| C | -1.27354200 | 0.63933000 | 0.10409000 |
| C | 1.11406300 | 0.71688000 | 0.13144700 |
| C | -1.33330800 | 1.96730100 | 0.44858900 |
| C | 1.06074900 | 2.04568600 | 0.48939200 |
| C | -0.16173700 | 2.68380500 | 0.75396500 |
| H | -2.29551200 | 2.46621700 | 0.42537200 |
| H | 1.98378500 | 2.61324400 | 0.49629000 |
| N | -0.05835800 | -0.07929400 | 0.10827200 |
| C | 0.49086400 | -2.53482000 | -0.30076200 |
| H | 1.57773900 | -2.49880700 | -0.37330900 |
| H | 0.21325100 | -3.52845900 | 0.06892100 |
| H | 0.06432900 | -2.41098900 | -1.29973500 |
| C | 0.51070000 | -1.53896200 | 2.07239000 |
| H | 0.37256800 | -2.54565700 | 2.48247900 |
| H | 1.57870300 | -1.31496400 | 2.07662700 |
| H | 0.00019200 | -0.83059700 | 2.73352700 |
| H | -0.19946200 | 3.72331100 | 1.05589200 |
| C | 2.39501400 | 0.16040600 | -0.42831500 |
| C | -2.51920400 | -0.06832600 | -0.35761700 |
| F | -3.45275000 | 0.80854600 | -0.78067800 |
| F | -2.26507800 | -0.92268700 | -1.37347100 |
| F | -3.11758700 | -0.80458600 | 0.62360200 |
| F | 2.19953200 | -0.41835900 | -1.63513800 |
| F | 3.31935700 | 1.13089500 | -0.58960000 |
| F | 2.98931900 | -0.78570000 | 0.35420000 |

**R'=Cl, R=iPr**
Zero-point correction= 0.164026 (Hartree/Particle)
Thermal correction to Energy= 0.175535
Thermal correction to Enthalpy= 0.176479
Thermal correction to Gibbs Free Energy= 0.125601
Sum of electronic and zero-point Energies= -1285.795120
Sum of electronic and thermal Energies= -1285.783611
Sum of electronic and thermal Enthalpies= -1285.782667
Sum of electronic and thermal Free Energies= -1285.833544
Single-point electronic energy (M06) = -1285.7695

| | | | |
|---|---|---|---|
| C | -0.23977500 | -1.49395300 | 0.58253100 |
| H | 0.73237500 | -1.84746600 | 0.93347500 |
| C | 1.38282700 | 0.31681600 | 0.01318100 |
| C | -0.90990100 | 0.85981700 | -0.09175300 |
| C | 1.70887300 | 1.61328500 | 0.30793500 |
| C | -0.63508000 | 2.17067000 | 0.20586600 |
| C | 0.68121800 | 2.55651300 | 0.52562800 |
| H | 2.75387700 | 1.90395100 | 0.31663000 |
| H | -1.43408500 | 2.90117700 | 0.13285400 |
| N | 0.06186000 | -0.14486500 | -0.01513600 |
| C | -1.15769400 | -1.38102800 | 1.80524100 |
| H | -2.16788500 | -1.06253100 | 1.53410000 |
| H | -1.23292800 | -2.36233200 | 2.28672600 |

| | | | |
|---|---|---|---|
| H | -0.75305500 | -0.67298400 | 2.53576100 |
| C | -0.74260800 | -2.49245100 | -0.46588700 |
| H | -0.79017700 | -3.49275700 | -0.01997800 |
| H | -1.73927400 | -2.23395100 | -0.83108300 |
| H | -0.05889400 | -2.53120600 | -1.31922800 |
| H | 0.90743300 | 3.56729300 | 0.84462900 |
| Cl | -2.46576400 | 0.44995200 | -0.83872600 |
| Cl | 2.63179000 | -0.80602000 | -0.54976700 |

**R'=tBu, R=iPr**

Zero-point correction= 0.409396 (Hartree/Particle)
Thermal correction to Energy= 0.429204
Thermal correction to Enthalpy= 0.430148
Thermal correction to Gibbs Free Energy= 0.363498
Sum of electronic and zero-point Energies= -680.846012
Sum of electronic and thermal Energies= -680.826204
Sum of electronic and thermal Enthalpies= -680.825260
Sum of electronic and thermal Free Energies= -680.891910
Single-point electronic energy (M06) = -680.90275

| | | | |
|---|---|---|---|
| C | -0.11855200 | -1.53219300 | 0.85471000 |
| H | -1.19237000 | -1.71135800 | 0.94479800 |
| C | -1.26963000 | 0.51588300 | 0.21550100 |
| C | 1.15672600 | 0.57137500 | 0.20008700 |
| C | -1.28903900 | 1.65689500 | 0.98354700 |
| C | 1.11408200 | 1.70659000 | 0.98236100 |
| C | -0.09689200 | 2.20647800 | 1.49744400 |
| H | -2.22719100 | 2.18416000 | 1.13580800 |
| H | 2.02190000 | 2.28093000 | 1.13839900 |
| N | -0.04429000 | -0.21900700 | 0.08785900 |
| C | 0.46050800 | -2.75923300 | 0.14222500 |
| H | 1.55067500 | -2.74566500 | 0.08468900 |
| H | 0.17839200 | -3.65716000 | 0.70555700 |
| H | 0.06335700 | -2.86065700 | -0.87128800 |
| C | 0.42017800 | -1.39041600 | 2.28600500 |
| H | 0.21215900 | -2.30621900 | 2.85225700 |
| H | 1.50119100 | -1.22331500 | 2.29815200 |
| H | -0.05876000 | -0.55160900 | 2.79923000 |
| H | -0.11320100 | 3.07988000 | 2.14101700 |
| C | 2.41113300 | 0.22869000 | -0.63702900 |
| C | -2.53113800 | 0.05547800 | -0.55256400 |
| C | -3.65983400 | -0.34565900 | 0.42740900 |
| H | -4.56927800 | -0.61510200 | -0.12434500 |
| H | -3.37416200 | -1.20778700 | 1.04129400 |
| H | -3.91120100 | 0.47563200 | 1.10690300 |
| C | -2.26434100 | -1.11493200 | -1.52026300 |
| H | -2.05646100 | -2.05438700 | -1.00147200 |
| H | -3.15325100 | -1.28001200 | -2.14030400 |
| H | -1.42018600 | -0.90071300 | -2.18219800 |
| C | -3.03203200 | 1.24476400 | -1.41565200 |
| H | -3.92603500 | 0.95288400 | -1.98155800 |
| H | -3.29375500 | 2.11393200 | -0.80473300 |
| H | -2.26342400 | 1.55824500 | -2.13080700 |
| C | 2.02499300 | -0.50246900 | -1.94108700 |
| H | 2.92403000 | -0.67483100 | -2.54526100 |
| H | 1.55028400 | -1.46685100 | -1.76417200 |
| H | 1.33162300 | 0.10468300 | -2.53371600 |
| C | 3.44902800 | -0.59962700 | 0.16136000 |
| H | 4.34799700 | -0.76943500 | -0.44466700 |
| H | 3.75225600 | -0.06336700 | 1.06808000 |
| H | 3.06984200 | -1.57773700 | 0.46704300 |
| C | 3.12687200 | 1.53601000 | -1.06914900 |
| H | 3.57046100 | 2.07180000 | -0.22377300 |
| H | 3.94426600 | 1.29414900 | -1.75904300 |
| H | 2.43848800 | 2.21715400 | -1.58032600 |

**R'=H, R=Et**

Zero-point correction= 0.154654 (Hartree/Particle)
Thermal correction to Energy= 0.162494
Thermal correction to Enthalpy= 0.163438
Thermal correction to Gibbs Free Energy= 0.121580
Sum of electronic and zero-point Energies= -327.310000
Sum of electronic and thermal Energies= -327.302161
Sum of electronic and thermal Enthalpies= -327.301216
Sum of electronic and thermal Free Energies= -327.343074
Single-point electronic energy (M06) = -327.29526

| | | | |
|---|---|---|---|
| C | 1.88823400 | 0.00000000 | -0.54730700 |
| H | 2.20087500 | 0.88027300 | -1.12190600 |
| C | -0.25423500 | 1.20340300 | -0.25978200 |
| C | -0.25423500 | -1.20340300 | -0.25978200 |
| C | -1.56766700 | 1.20953100 | 0.11598200 |
| C | -1.56766700 | -1.20953100 | 0.11598200 |
| C | -2.28101800 | 0.00000000 | 0.32161200 |
| H | -2.05790100 | 2.17026700 | 0.24785600 |
| H | -2.05790000 | -2.17026700 | 0.24785600 |
| N | 0.43255200 | 0.00000000 | -0.49068000 |
| C | 2.56419900 | 0.00000000 | 0.82987100 |
| H | 2.27339100 | -0.88580600 | 1.40493400 |
| H | 3.65544000 | 0.00000100 | 0.72438400 |
| H | 2.27338900 | 0.88580400 | 1.40493500 |
| H | -3.31966200 | 0.00000000 | 0.62875200 |
| H | 2.20087500 | -0.88027200 | -1.12190700 |
| H | 0.31898200 | -2.10587600 | -0.43980600 |
| H | 0.31898200 | 2.10587600 | -0.43980600 |

**R'=Me, R=Et**

Zero-point correction= 0.211731 (Hartree/Particle)
Thermal correction to Energy= 0.222204
Thermal correction to Enthalpy= 0.223148
Thermal correction to Gibbs Free Energy= 0.175790
Sum of electronic and zero-point Energies= -405.886414
Sum of electronic and thermal Energies= -405.875941
Sum of electronic and thermal Enthalpies= -405.874997
Sum of electronic and thermal Free Energies= -405.922354
Single-point electronic energy (M06) = -405.88515

| | | | |
|---|---|---|---|
| C | 1.80037600 | 0.00167700 | -0.29863700 |
| H | 2.17960900 | -0.87051000 | -0.83583300 |
| C | -0.36001500 | -1.22275100 | -0.18806800 |
| C | -0.36244700 | 1.22197500 | -0.18807200 |
| C | -1.66512900 | -1.20609500 | 0.23105200 |
| C | -1.66753600 | 1.20284700 | 0.23094900 |
| C | -2.36027700 | -0.00235000 | 0.48426200 |
| H | -2.17070900 | -2.16171100 | 0.34340900 |
| H | -2.17500700 | 2.15745600 | 0.34325600 |
| N | 0.33609700 | 0.00034800 | -0.39059200 |
| C | 2.33224500 | 0.00236000 | 1.14182300 |
| H | 3.42886200 | 0.00313600 | 1.14635100 |
| H | 1.98559800 | 0.88632700 | 1.68770400 |
| H | 1.98685700 | -0.88194600 | 1.68796400 |
| H | -3.38819600 | -0.00337300 | 0.82678500 |
| C | 0.34442400 | 2.50362900 | -0.53013800 |
| H | 1.21666600 | 2.70640000 | 0.10706200 |
| H | 0.69958100 | 2.51288000 | -1.57106100 |
| H | -0.34724500 | 3.34166700 | -0.40967800 |
| C | 0.34950400 | -2.50287600 | -0.53015600 |
| H | 1.22194400 | -2.70406800 | 0.10732500 |
| H | -0.34055500 | -3.34231400 | -0.41013900 |
| H | 0.70505700 | -2.51125400 | -1.57093500 |
| H | 2.17799500 | 0.87437400 | -0.83614800 |

**R'=Ph, R=Et**

Zero-point correction= 0.317841 (Hartree/Particle)
Thermal correction to Energy= 0.334567
Thermal correction to Enthalpy= 0.335511
Thermal correction to Gibbs Free Energy= 0.272122
Sum of electronic and zero-point Energies= -789.262221
Sum of electronic and thermal Energies= -789.245494
Sum of electronic and thermal Enthalpies= -789.244550
Sum of electronic and thermal Free Energies= -789.307940
Single-point electronic energy (M06) = -789.16035

| | | | |
|---|---|---|---|
| C | -0.00000800 | -0.52456500 | 1.43432800 |
| H | -0.87910900 | -1.17054400 | 1.45631300 |
| C | -1.22022700 | 0.83582700 | -0.22921100 |
| C | 1.22022900 | 0.83583300 | -0.22920900 |
| C | -1.20499800 | 2.14174500 | -0.67505300 |
| C | 1.20502500 | 2.14171700 | -0.67508500 |

| | | | |
|---|---|---|---|
| C | -0.00000800 | 2.84717400 | -0.84514100 |
| H | -2.14511000 | 2.59188200 | -0.97908600 |
| H | 2.14509000 | 2.59188900 | -0.97918900 |
| N | 0.00003300 | 0.20401000 | 0.13708700 |
| C | -2.45537500 | 0.03409000 | -0.20507200 |
| C | -3.68964000 | 0.61521700 | 0.14830200 |
| C | -2.44851000 | -1.32912500 | -0.56582900 |
| C | -4.86627300 | -0.12927900 | 0.12463000 |
| H | -3.71688900 | 1.65459800 | 0.46350000 |
| C | -3.62614100 | -2.07198300 | -0.58366600 |
| H | -1.51019800 | -1.79135300 | -0.85902900 |
| C | -4.84316400 | -1.47793600 | -0.23944200 |
| H | -5.80440900 | 0.34274100 | 0.40534600 |
| H | -3.59508900 | -3.11837400 | -0.87693500 |
| H | -5.76083300 | -2.05947700 | -0.25074500 |
| C | 2.45543500 | 0.03409800 | -0.20506400 |
| C | 2.44859700 | -1.32909000 | -0.56589500 |
| C | 3.68965500 | 0.61521400 | 0.14845600 |
| C | 3.62624900 | -2.07192100 | -0.58373000 |
| H | 1.51031200 | -1.79133000 | -0.85915400 |
| C | 4.86630900 | -0.12925900 | 0.12480000 |
| H | 3.71685600 | 1.65456100 | 0.46376500 |
| C | 4.84324100 | -1.47788000 | -0.23939200 |
| H | 3.59523700 | -3.11828900 | -0.87708700 |
| H | 5.80440900 | 0.34275000 | 0.40565700 |
| H | 5.76091900 | -2.05940600 | -0.25072200 |
| C | -0.00033600 | 0.41599400 | 2.64191000 |
| H | -0.00025500 | -0.16526300 | 3.57137600 |
| H | 0.88698700 | 1.05796700 | 2.63990700 |
| H | -0.88796000 | 1.05755200 | 2.63977900 |
| H | 0.00003800 | 3.86694000 | -1.21368800 |
| H | 0.87941500 | -1.17013000 | 1.45655200 |

**R'=CF3, R=Et**

Zero-point correction= 0.166003 (Hartree/Particle)
Thermal correction to Energy= 0.180267
Thermal correction to Enthalpy= 0.181211
Thermal correction to Gibbs Free Energy= 0.124015
Sum of electronic and zero-point Energies= -1001.370311
Sum of electronic and thermal Energies= -1001.356046
Sum of electronic and thermal Enthalpies= -1001.355102
Sum of electronic and thermal Free Energies= -1001.412299
Single-point electronic energy (M06) = -1001.3557

| | | | |
|---|---|---|---|
| C | 0.00007100 | -1.63274200 | -0.10980000 |
| H | 0.87082300 | -2.03062800 | 0.40818100 |
| C | 1.20181700 | 0.57080500 | -0.06073300 |
| C | -1.20183400 | 0.57076200 | -0.06075400 |
| C | 1.20072600 | 1.88951700 | -0.44317300 |
| C | -1.20077500 | 1.88947700 | -0.44318800 |
| C | -0.00003400 | 2.57630100 | -0.69873800 |
| H | 2.15230000 | 2.40285800 | -0.50986600 |
| H | -2.15236500 | 2.40278900 | -0.50988500 |
| N | 0.00000600 | -0.16177500 | 0.07367200 |
| C | 0.00010100 | -2.05975700 | -1.57999600 |
| H | 0.00016700 | -3.15395000 | -1.64324900 |
| H | -0.89038300 | -1.68920200 | -2.09500700 |
| H | 0.89054400 | -1.68909500 | -2.09500000 |
| H | -0.00004900 | 3.61239600 | -1.01308900 |
| C | -2.49063900 | -0.10522300 | 0.30625200 |
| C | 2.49062100 | -0.10518100 | 0.30626500 |
| H | -0.87063000 | -2.03072900 | 0.40818400 |
| F | -3.51390000 | 0.77005300 | 0.33999500 |
| F | -2.42525800 | -0.70123200 | 1.52290200 |
| F | -2.85146700 | -1.08307700 | -0.57195600 |
| F | 2.42523300 | -0.70118500 | 1.52291600 |
| F | 2.85141000 | -1.08305700 | -0.57193300 |
| F | 3.51389900 | 0.77007900 | 0.33999100 |

**R'=Cl, R=Et**

Zero-point correction= 0.135947 (Hartree/Particle)
Thermal correction to Energy= 0.146085
Thermal correction to Enthalpy= 0.147029
Thermal correction to Gibbs Free Energy= 0.098520
Sum of electronic and zero-point Energies= -1246.512837
Sum of electronic and thermal Energies= -1246.502700
Sum of electronic and thermal Enthalpies= -1246.501755
Sum of electronic and thermal Free Energies= -1246.550264
Single-point electronic energy (M06) = -1246.4793

| | | | |
|---|---|---|---|
| C | 0.00003500 | -1.77594600 | 0.15321100 |
| H | 0.87946300 | -2.22470600 | -0.31162700 |
| C | 1.18425600 | 0.40297300 | -0.07669900 |
| C | -1.18418200 | 0.40297500 | -0.07669500 |
| C | 1.20766600 | 1.68610000 | 0.39867600 |
| C | -1.20759400 | 1.68612900 | 0.39867200 |
| C | 0.00002500 | 2.33195500 | 0.74073900 |
| H | 2.15951000 | 2.20252800 | 0.46108600 |
| H | -2.15945700 | 2.20252200 | 0.46108300 |
| N | 0.00002000 | -0.33822700 | -0.21023700 |
| C | -0.00024200 | -2.00839100 | 1.66506500 |
| H | -0.88829600 | -1.56746900 | 2.13025100 |
| H | -0.00009400 | -3.08316800 | 1.87906600 |
| H | 0.88748400 | -1.56716800 | 2.13060500 |
| H | 0.00005200 | 3.31737900 | 1.19110800 |
| Cl | -2.64700500 | -0.32471900 | -0.74639000 |
| Cl | 2.64704100 | -0.32482900 | -0.74630300 |
| H | -0.87920300 | -2.22477400 | -0.31195500 |

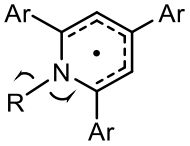
**R'=tBu, R=Et**

Zero-point correction= 0.381522 (Hartree/Particle)
Thermal correction to Energy= 0.400062
Thermal correction to Enthalpy= 0.401006
Thermal correction to Gibbs Free Energy= 0.336250
Sum of electronic and zero-point Energies= -641.571756
Sum of electronic and thermal Energies= -641.553216
Sum of electronic and thermal Enthalpies= -641.552272
Sum of electronic and thermal Free Energies= -641.617028
Single-point electronic energy (M06) = -641.62025

| | | | |
|---|---|---|---|
| C | 0.00001900 | -1.52132600 | 0.88458100 |
| H | 0.87153000 | -2.10808400 | 0.59356700 |
| C | -1.22559400 | 0.47883900 | 0.10395400 |
| C | 1.22558200 | 0.47886200 | 0.10395800 |
| C | -1.20521300 | 1.77246700 | 0.57111000 |
| C | 1.20516500 | 1.77248700 | 0.57115100 |
| C | -0.00002000 | 2.41245400 | 0.92474900 |
| H | -2.12891000 | 2.33996100 | 0.60665900 |
| H | 2.12889100 | 2.33993700 | 0.60675700 |
| N | -0.00002100 | -0.26254300 | 0.09822900 |
| C | 0.00040300 | -1.29961400 | 2.40061400 |
| H | -0.88554200 | -0.73801700 | 2.71408000 |
| H | 0.00061700 | -2.26293300 | 2.92507300 |
| H | 0.88640100 | -0.73786500 | 2.71363700 |
| H | -0.00004500 | 3.42168900 | 1.32214300 |
| C | 2.49615300 | -0.16655700 | -0.49248400 |
| C | -2.49622000 | -0.16659700 | -0.49238400 |
| C | -3.33639300 | -0.91989300 | 0.57337300 |
| H | -4.27496700 | -1.27700700 | 0.13091200 |
| H | -2.82033200 | -1.78952800 | 0.99019200 |
| H | -3.58880500 | -0.25198300 | 1.40455300 |
| C | -2.13522000 | -1.11778600 | -1.65709100 |
| H | -1.51653800 | -1.96274400 | -1.34599200 |
| H | -3.05280100 | -1.52335100 | -2.09986900 |
| H | -1.58943100 | -0.58108500 | -2.44056400 |
| C | -3.41682500 | 0.92960800 | -1.08619800 |
| H | -4.25954500 | 0.45848800 | -1.60598600 |
| H | -3.84076800 | 1.57997300 | -0.31426800 |
| H | -2.87968900 | 1.55722700 | -1.80491700 |
| C | 2.13501800 | -1.11716700 | -1.65761100 |
| H | 3.05249900 | -1.52314900 | -2.10020400 |
| H | 1.51563900 | -1.96179400 | -1.34701100 |
| H | 1.58985900 | -0.57983900 | -2.44110200 |
| C | 3.33612200 | -0.92045200 | 0.57300600 |
| H | 4.27477400 | -1.27730700 | 0.13050100 |
| H | 3.58841600 | -0.25304300 | 1.40463100 |
| H | 2.81999500 | -1.79033200 | 0.98921300 |

| | | | |
|---|---|---|---|
| C | 3.41701900 | 0.92972700 | -1.08576100 |
| H | 3.84092100 | 1.57975400 | -0.31351800 |
| H | 4.25973800 | 0.45867700 | -1.60561500 |
| H | 2.88007300 | 1.55767100 | -1.80433600 |
| H | -0.87180900 | -2.10782900 | 0.59405900 |

## Dissociation Transition States




**Ar=Ph, R=Cy**

Zero-point correction= 0.490520 (Hartree/Particle)
Thermal correction to Energy= 0.515381
Thermal correction to Enthalpy= 0.516325
Thermal correction to Gibbs Free Energy= 0.432964
Sum of electronic and zero-point Energies= -1176.166291
Sum of electronic and thermal Energies= -1176.141431
Sum of electronic and thermal Enthalpies= -1176.140487
Sum of electronic and thermal Free Energies= -1176.223848
Single-point electronic energy (M06) = -1176.03771012

| | | | |
|---|---|---|---|
| C | 0.27214500 | 1.31682900 | -0.48976900 |
| C | -0.02329700 | -1.00245700 | -0.67280600 |
| C | 1.62995500 | 1.14583300 | -0.24463600 |
| C | 1.32729500 | -1.21598700 | -0.41760700 |
| C | 2.19753900 | -0.13942200 | -0.16371300 |
| H | 2.26398700 | 2.02049700 | -0.14926700 |
| H | 1.73113800 | -2.21787300 | -0.51870900 |
| N | -0.58870300 | 0.24939500 | -0.61585300 |
| C | -0.32288100 | 2.66680600 | -0.64050400 |
| C | 0.23323400 | 3.79818100 | -0.01562600 |
| C | -1.47234800 | 2.84580700 | -1.43174700 |
| C | -0.32838400 | 5.06149800 | -0.18949700 |
| H | 1.09721700 | 3.68583400 | 0.63305000 |
| C | -2.03263300 | 4.10950000 | -1.60507700 |
| H | -1.90916300 | 1.97933200 | -1.91644200 |
| C | -1.46298600 | 5.22500100 | -0.98719900 |
| H | 0.11587200 | 5.91931500 | 0.30880700 |
| H | -2.91506000 | 4.22478300 | -2.22947500 |
| C | -0.90868800 | -2.12195700 | -1.07877200 |
| C | -1.95831700 | -1.89804600 | -1.98726600 |
| C | -0.70911600 | -3.43099400 | -0.60510300 |
| C | -2.77219400 | -2.94586700 | -2.41226200 |
| H | -2.11686200 | -0.89154700 | -2.35976200 |
| C | -1.52568400 | -4.47848300 | -1.02816900 |
| H | 0.07785900 | -3.62600400 | 0.11821300 |
| C | -2.56054500 | -4.24184100 | -1.93517700 |
| H | -3.57172600 | -2.75163600 | -3.12276100 |
| H | -1.35772800 | -5.48049200 | -0.64181600 |
| C | 3.63469300 | -0.35030500 | 0.10476700 |
| C | 4.07763100 | -1.50152300 | 0.78349700 |
| C | 4.60477200 | 0.58407500 | -0.30510100 |
| C | 5.43105200 | -1.71046300 | 1.04003300 |
| H | 3.34839600 | -2.22498100 | 1.13717100 |
| C | 5.95763200 | 0.37576000 | -0.04672200 |
| H | 4.29844300 | 1.46709400 | -0.85865500 |
| C | 6.37949600 | -0.77264000 | 0.62729900 |
| H | 5.74464800 | -2.60448400 | 1.57296300 |
| H | 6.68671300 | 1.10871400 | -0.38258500 |
| C | -1.88535800 | 0.38830900 | 1.04915100 |
| C | -3.28387300 | -0.00760200 | 0.66723700 |
| C | -1.26124900 | -0.43957500 | 2.13610200 |
| H | -1.73381400 | 1.46131900 | 1.14840300 |
| C | -4.19062300 | 0.03058900 | 1.92558500 |
| H | -3.29201400 | -1.02712900 | 0.26310000 |
| H | -3.68060500 | 0.65518800 | -0.11001000 |
| C | -2.16459000 | -0.41615600 | 3.39629600 |
| H | -1.16099300 | -1.48138000 | 1.80028200 |
| H | -0.25578200 | -0.07813100 | 2.38191400 |
| C | -3.60499900 | -0.83018800 | 3.05620100 |
| H | -5.20061500 | -0.31243000 | 1.66487400 |
| H | -4.28930300 | 1.06953300 | 2.27125200 |
| H | -1.74484300 | -1.07799600 | 4.16551200 |
| H | -2.16667500 | 0.59811500 | 3.81990600 |
| H | -4.23784900 | -0.76139800 | 3.95046000 |
| H | -3.61340000 | -1.88565800 | 2.74644700 |
| H | -3.19698100 | -5.05847100 | -2.26529500 |
| H | 7.43500700 | -0.93436700 | 0.82826400 |
| H | -1.90102400 | 6.21040600 | -1.12136200 |

**Ar=4-Me-Ph, R=Cy**

Zero-point correction= 0.573013 (Hartree/Particle)
Thermal correction to Energy= 0.603623
Thermal correction to Enthalpy= 0.604567
Thermal correction to Gibbs Free Energy= 0.506387
Sum of electronic and zero-point Energies= -1294.038232
Sum of electronic and thermal Energies= -1294.007622
Sum of electronic and thermal Enthalpies= -1294.006678
Sum of electronic and thermal Free Energies= -1294.104858
Single-point electronic energy (M06) = -1293.92240646

| | | | |
|---|---|---|---|
| C | 0.12004500 | 1.30090200 | -0.42953800 |
| C | -0.08994400 | -1.03402600 | -0.52397900 |
| C | 1.49773600 | 1.19241000 | -0.27975500 |
| C | 1.28372700 | -1.18413000 | -0.36190100 |
| C | 2.12392100 | -0.06599900 | -0.20474200 |
| H | 2.09894200 | 2.09477900 | -0.25732000 |
| H | 1.72190000 | -2.17144000 | -0.46405100 |
| N | -0.70209000 | 0.19626700 | -0.46232500 |
| C | -0.54001500 | 2.61980300 | -0.57487200 |
| C | 0.00505600 | 3.79356600 | -0.02269900 |
| C | -1.74326000 | 2.73646900 | -1.29161300 |
| C | -0.61866500 | 5.02549600 | -0.19461500 |
| H | 0.91550500 | 3.74005800 | 0.56755200 |
| C | -2.36171200 | 3.97294400 | -1.46051200 |
| H | -2.17773800 | 1.84387400 | -1.72894200 |
| C | -1.81488400 | 5.14211100 | -0.91688200 |
| H | -0.17291500 | 5.91372400 | 0.24865300 |
| H | -3.28543800 | 4.03268600 | -2.03245500 |
| C | -0.95369600 | -2.19944900 | -0.83253300 |
| C | -2.08072300 | -2.05024700 | -1.65971000 |
| C | -0.66318600 | -3.48867900 | -0.35467100 |
| C | -2.87370700 | -3.14311500 | -1.99636500 |
| H | -2.31630300 | -1.06413400 | -2.04592400 |
| C | -1.46260700 | -4.57844600 | -0.69296600 |
| H | 0.18746500 | -3.63935800 | 0.30446400 |
| C | -2.58409500 | -4.42932800 | -1.51843500 |
| H | -3.73173200 | -2.99768100 | -2.64976900 |
| H | -1.21375300 | -5.56291200 | -0.30229500 |
| C | 3.58460800 | -0.20953500 | -0.04523000 |
| C | 4.13560700 | -1.31783600 | 0.62451600 |
| C | 4.48168200 | 0.74914400 | -0.55082700 |
| C | 5.51198800 | -1.45866600 | 0.77727800 |
| H | 3.47397600 | -2.06241000 | 1.05851900 |
| C | 5.85718400 | 0.60318300 | -0.39433000 |
| H | 4.10002200 | 1.60711300 | -1.09714100 |
| C | 6.40282800 | -0.50382500 | 0.26914900 |
| H | 5.90214800 | -2.32263900 | 1.31151700 |
| H | 6.52201700 | 1.36078900 | -0.80412100 |
| C | -1.89425000 | 0.33911000 | 1.27119300 |
| C | -3.31050200 | -0.05843000 | 0.96111900 |
| C | -1.21684400 | -0.48494400 | 2.32951000 |
| H | -1.73937600 | 1.41261900 | 1.36124100 |
| C | -4.15450700 | -0.02089300 | 2.26153200 |
| H | -3.33513800 | -1.07778200 | 0.55731400 |
| H | -3.74553000 | 0.60329300 | 0.20374800 |
| C | -2.05809300 | -0.46035800 | 3.63187600 |
| H | -1.13032600 | -1.52721000 | 1.99194400 |
| H | -0.20132000 | -0.12106400 | 2.52567100 |
| C | -3.51246200 | -0.87846700 | 3.36349800 |
| H | -5.17564800 | -0.36617300 | 2.05176800 |

| | | | |
|---|---|---|---|
| H | -4.23820200 | 1.01831200 | 2.61057400 |
| H | -1.60013700 | -1.11895300 | 4.38194400 |
| H | -2.04274000 | 0.55517700 | 4.05232200 |
| H | -4.10063700 | -0.80926000 | 4.28779400 |
| H | -3.53349400 | -1.93463100 | 3.05677900 |
| C | -3.46708600 | -5.60583400 | -1.86146000 |
| H | -4.33546800 | -5.66369800 | -1.19096500 |
| H | -3.85483500 | -5.53155000 | -2.88359000 |
| H | -2.92526000 | -6.55344700 | -1.77360500 |
| C | -2.49907500 | 6.47907000 | -1.07815900 |
| H | -3.23199700 | 6.45756800 | -1.89126900 |
| H | -3.03351700 | 6.76854900 | -0.16319500 |
| H | -1.77853000 | 7.27629700 | -1.29437200 |
| C | 7.89688900 | -0.67554900 | 0.40903900 |
| H | 8.15717100 | -1.18143500 | 1.34534700 |
| H | 8.30855900 | -1.28077800 | -0.41027800 |
| H | 8.41521400 | 0.28913800 | 0.39093100 |

**Ar=4-MeO-Ph, R=Cy**

Zero-point correction= 0.588631 (Hartree/Particle)
Thermal correction to Energy= 0.621396
Thermal correction to Enthalpy= 0.622341
Thermal correction to Gibbs Free Energy= 0.520749
Sum of electronic and zero-point Energies= -1519.636610
Sum of electronic and thermal Energies= -1519.603845
Sum of electronic and thermal Enthalpies= -1519.602901
Sum of electronic and thermal Free Energies= -1519.704492
Single-point electronic energy (M06) = -1519.52298931

| | | | |
|---|---|---|---|
| C | -0.09409500 | 1.32279300 | -0.34423500 |
| C | 0.00065600 | -1.02196600 | -0.41354900 |
| C | 1.29367800 | 1.39773600 | -0.30787200 |
| C | 1.39042600 | -0.98686500 | -0.36866400 |
| C | 2.08573500 | 0.23424700 | -0.28001500 |
| H | 1.77036800 | 2.37145400 | -0.33954600 |
| H | 1.94596300 | -1.90808300 | -0.51104500 |
| N | -0.76306000 | 0.11760100 | -0.29729500 |
| C | -0.93301900 | 2.53894900 | -0.44275500 |
| C | -0.50005800 | 3.79253700 | 0.03612100 |
| C | -2.20344100 | 2.48041000 | -1.03592100 |
| C | -1.28857000 | 4.92659700 | -0.08734200 |
| H | 0.46025700 | 3.87736600 | 0.53640400 |
| C | -3.00802600 | 3.61249900 | -1.16772500 |
| H | -2.55699900 | 1.52605700 | -1.41122200 |
| C | -2.55120300 | 4.84805700 | -0.69429100 |
| H | -0.95383500 | 5.88766600 | 0.29077000 |
| H | -3.97823100 | 3.52074300 | -1.64327300 |
| C | -0.72288100 | -2.29431000 | -0.64436900 |
| C | -1.92823000 | -2.31022300 | -1.36105200 |
| C | -0.22119400 | -3.53162200 | -0.19319800 |
| C | -2.60999100 | -3.49767200 | -1.62904300 |
| H | -2.33071900 | -1.36914200 | -1.72078700 |
| C | -0.88804100 | -4.72079600 | -0.44938800 |
| H | 0.69578100 | -3.55918800 | 0.38874100 |
| C | -2.09019300 | -4.71506700 | -1.17250900 |
| H | -3.53362500 | -3.46250500 | -2.19591800 |
| H | -0.50321200 | -5.67041900 | -0.09046500 |
| C | 3.55969000 | 0.28637200 | -0.23532500 |
| C | 4.30468800 | -0.73463100 | 0.37587700 |
| C | 4.28325100 | 1.35654900 | -0.80282800 |
| C | 5.69921500 | -0.70623700 | 0.42562700 |
| H | 3.78498500 | -1.56226700 | 0.85040000 |
| C | 5.66817900 | 1.40037400 | -0.76045500 |
| H | 3.75077200 | 2.15370200 | -1.31338600 |
| C | 6.39149600 | 0.36759100 | -0.14476500 |
| H | 6.22821600 | -1.51438000 | 0.91813700 |
| H | 6.21821800 | 2.22141000 | -1.21006600 |
| C | -1.79323100 | 0.12237900 | 1.52626700 |
| C | -3.16121200 | -0.47860200 | 1.35671300 |
| C | -0.91226200 | -0.57192500 | 2.52736800 |
| H | -1.79035800 | 1.20838000 | 1.59844100 |
| C | -3.88024500 | -0.52901900 | 2.72969000 |
| H | -3.07928400 | -1.50127500 | 0.96897500 |
| H | -3.75392700 | 0.09658000 | 0.63613600 |
| C | -1.62682200 | -0.63705500 | 3.90200400 |
| H | -0.70563600 | -1.59914600 | 2.19517500 |
| H | 0.05330100 | -0.06157300 | 2.62413200 |
| C | -3.02463000 | -1.26235700 | 3.77469700 |
| H | -4.85708900 | -1.01917200 | 2.62071500 |
| H | -4.07825900 | 0.49596500 | 3.07488100 |
| H | -1.01361500 | -1.20759600 | 4.61243800 |
| H | -1.71786900 | 0.37956600 | 4.31027400 |
| H | -3.53002000 | -1.25713800 | 4.74921600 |
| H | -2.92236500 | -2.31726900 | 3.48005000 |
| O | 7.75045300 | 0.50433100 | -0.15586400 |
| O | -3.24969800 | 6.01917300 | -0.76720900 |
| O | -2.66971400 | -5.93533400 | -1.37195500 |
| C | 8.53115600 | -0.51600900 | 0.44395900 |
| H | 9.57176200 | -0.21197400 | 0.31583300 |
| H | 8.31274300 | -0.61548800 | 1.51573400 |
| H | 8.37431400 | -1.48637200 | -0.04595600 |
| C | -3.89105600 | -5.98784800 | -2.09079800 |
| H | -3.77461400 | -5.60832100 | -3.11471300 |
| H | -4.17206000 | -7.04207200 | -2.12759300 |
| H | -4.68286000 | -5.41922700 | -1.58495900 |
| C | -4.53413600 | 5.99660700 | -1.36786100 |
| H | -4.90559300 | 7.02199800 | -1.31995000 |
| H | -4.48407100 | 5.67824700 | -2.41766500 |
| H | -5.22314200 | 5.33594100 | -0.82480100 |

**Ar=4-CF3-Ph, R=Cy**

Zero-point correction= 0.504496 (Hartree/Particle)
Thermal correction to Energy= 0.540501
Thermal correction to Enthalpy= 0.541445
Thermal correction to Gibbs Free Energy= 0.427898
Sum of electronic and zero-point Energies= -2187.265827
Sum of electronic and thermal Energies= -2187.229822
Sum of electronic and thermal Enthalpies= -2187.228878
Sum of electronic and thermal Free Energies= -2187.342425
Single-point electronic energy (M06) = -2187.14485341

| | | | |
|---|---|---|---|
| C | -0.15592300 | 1.27274700 | -0.24568200 |
| C | -0.18689200 | -1.06941100 | -0.24872900 |
| C | 1.23379900 | 1.27799300 | -0.20611400 |
| C | 1.20272600 | -1.11025600 | -0.19257100 |
| C | 1.96019400 | 0.07443000 | -0.14336600 |
| H | 1.76153400 | 2.22373100 | -0.25922000 |
| H | 1.70868300 | -2.06442000 | -0.29485900 |
| N | -0.88711200 | 0.10987900 | -0.18234200 |
| C | -0.92796900 | 2.53105500 | -0.37947500 |
| C | -0.43137700 | 3.76204400 | 0.09136500 |
| C | -2.19121800 | 2.51961600 | -0.99543100 |
| C | -1.16165300 | 4.93392000 | -0.06224500 |
| H | 0.52313000 | 3.79983600 | 0.60721200 |
| C | -2.92505600 | 3.69235300 | -1.15276300 |
| H | -2.58464700 | 1.57804000 | -1.36144300 |
| C | -2.41299400 | 4.90467700 | -0.68812100 |
| H | -0.76762800 | 5.87280000 | 0.31532700 |
| H | -3.89378500 | 3.66714000 | -1.63972200 |
| C | -0.97597100 | -2.30884200 | -0.45164000 |
| C | -2.17494300 | -2.27069800 | -1.18497100 |
| C | -0.54380500 | -3.55082600 | 0.04778500 |
| C | -2.90857400 | -3.42872800 | -1.42057400 |
| H | -2.51849700 | -1.31880300 | -1.57429800 |
| C | -1.27592100 | -4.71098300 | -0.18264300 |
| H | 0.36076000 | -3.60667300 | 0.64594800 |
| C | -2.46210200 | -4.65512200 | -0.91977700 |
| H | -3.82966000 | -3.38248600 | -1.99237600 |
| H | -0.93626300 | -5.65832100 | 0.22333600 |
| C | 3.43544100 | 0.04807700 | -0.10110600 |
| C | 4.11792200 | -0.99195200 | 0.55858100 |
| C | 4.20687700 | 1.05394500 | -0.71379900 |
| C | 5.50736900 | -1.02942900 | 0.60164900 |
| H | 3.55122500 | -1.76412000 | 1.07006400 |

| | | | |
|---|---|---|---|
| C | 5.59618500 | 1.02144400 | -0.67188900 |
| H | 3.71515100 | 1.85617800 | -1.25522600 |
| C | 6.25445600 | -0.02135600 | -0.01349600 |
| H | 6.01360400 | -1.83215800 | 1.12785000 |
| H | 6.17238500 | 1.80454900 | -1.15385100 |
| C | -1.96471000 | 0.22768100 | 1.66854500 |
| C | -3.36452200 | -0.27799500 | 1.47402800 |
| C | -1.14617400 | -0.51428600 | 2.68429500 |
| H | -1.87316300 | 1.31135400 | 1.70703000 |
| C | -4.10855400 | -0.26396900 | 2.83628600 |
| H | -3.34480200 | -1.30878800 | 1.10012700 |
| H | -3.90335000 | 0.32800100 | 0.73743400 |
| C | -1.88810700 | -0.51427000 | 4.04828000 |
| H | -1.00902700 | -1.55731300 | 2.36633600 |
| H | -0.14928600 | -0.07127200 | 2.79300900 |
| C | -3.32318300 | -1.04318600 | 3.90248400 |
| H | -5.11345600 | -0.68712200 | 2.71072400 |
| H | -4.24227900 | 0.77574000 | 3.16660200 |
| H | -1.32503400 | -1.11754800 | 4.77217700 |
| H | -1.91437200 | 0.51056400 | 4.44409100 |
| H | -3.84225400 | -0.98959900 | 4.86778300 |
| H | -3.29065900 | -2.10632500 | 3.62283400 |
| C | -3.22069800 | -5.91846300 | -1.21813600 |
| C | 7.75589000 | -0.08962200 | -0.01985000 |
| C | -3.17617900 | 6.18993500 | -0.84734900 |
| F | 8.23709300 | -0.71150900 | 1.08020900 |
| F | 8.22327000 | -0.77462600 | -1.09103800 |
| F | 8.31569100 | 1.14015600 | -0.06948900 |
| F | -2.76120700 | -6.52672800 | -2.33738100 |
| F | -3.11273100 | -6.81849500 | -0.21423300 |
| F | -4.53740300 | -5.68332200 | -1.41316800 |
| F | -4.39059400 | 6.00252000 | -1.40604400 |
| F | -2.50676300 | 7.07235900 | -1.62630600 |
| F | -3.37008200 | 6.80239100 | 0.34501400 |

**Ar=4-F-Ph, R=Cy**

Zero-point correction= 0.465726 (Hartree/Particle)
Thermal correction to Energy= 0.493168
Thermal correction to Enthalpy= 0.494112
Thermal correction to Gibbs Free Energy= 0.404635
Sum of electronic and zero-point Energies= -1473.891076
Sum of electronic and thermal Energies= -1473.863633
Sum of electronic and thermal Enthalpies= -1473.862689
Sum of electronic and thermal Free Energies= -1473.952167
Single-point electronic energy (M06) = -1473.76156402

| | | | |
|---|---|---|---|
| C | 0.12537900 | 1.30057300 | -0.43099900 |
| C | -0.09533800 | -1.03217000 | -0.53369100 |
| C | 1.50152700 | 1.18544800 | -0.27414900 |
| C | 1.27638400 | -1.19020100 | -0.36574200 |
| C | 2.12072400 | -0.07639100 | -0.19971400 |
| H | 2.10753000 | 2.08458900 | -0.24650200 |
| H | 1.71080200 | -2.17888400 | -0.47179700 |
| N | -0.70267300 | 0.20045400 | -0.47022000 |
| C | -0.52836400 | 2.62277700 | -0.57718800 |
| C | 0.01825100 | 3.79016200 | -0.01252400 |
| C | -1.72764200 | 2.74032700 | -1.30431900 |
| C | -0.59338500 | 5.03039000 | -0.17843400 |
| H | 0.92112200 | 3.72851200 | 0.58741500 |
| C | -2.35126400 | 3.97288000 | -1.47866600 |
| H | -2.15979100 | 1.84779800 | -1.74288900 |
| C | -1.77127100 | 5.10307200 | -0.91346000 |
| H | -0.17912400 | 5.93145000 | 0.26198700 |
| H | -3.27023100 | 4.06981100 | -2.04785500 |
| C | -0.96404100 | -2.19160500 | -0.85152500 |
| C | -2.08207400 | -2.02834300 | -1.68939700 |
| C | -0.68492300 | -3.48200200 | -0.36601600 |
| C | -2.88931000 | -3.10784700 | -2.03809800 |
| H | -2.30567000 | -1.03878300 | -2.07252700 |
| C | -1.48354800 | -4.57249200 | -0.70408400 |
| H | 0.15598100 | -3.63459600 | 0.30412200 |
| C | -2.57595600 | -4.36755100 | -1.53883200 |
| H | -3.74728800 | -2.98904700 | -2.69201000 |
| H | -1.27756300 | -5.56771400 | -0.32383600 |
| C | 3.58011800 | -0.22729000 | -0.03296900 |
| C | 4.11756400 | -1.33639100 | 0.64815100 |
| C | 4.48177700 | 0.72403200 | -0.54825500 |
| C | 5.49160100 | -1.49599400 | 0.81027200 |
| H | 3.44772900 | -2.07308800 | 1.08153200 |
| C | 5.85784400 | 0.58071800 | -0.39252700 |
| H | 4.10406400 | 1.57540400 | -1.10641400 |
| C | 6.34382900 | -0.53109100 | 0.28651700 |
| H | 5.90579600 | -2.34580600 | 1.34304700 |
| H | 6.55379100 | 1.30743400 | -0.79892500 |
| C | -1.89887600 | 0.34187500 | 1.26235700 |
| C | -3.31163000 | -0.07083700 | 0.95712900 |
| C | -1.21260300 | -0.46758900 | 2.32579700 |
| H | -1.75410400 | 1.41740200 | 1.34509900 |
| C | -4.15390900 | -0.02564100 | 2.25881800 |
| H | -3.32897400 | -1.09531600 | 0.56604400 |
| H | -3.75400800 | 0.57823800 | 0.19305300 |
| C | -2.05198400 | -0.43643800 | 3.62963700 |
| H | -1.11972900 | -1.51244200 | 1.99781500 |
| H | -0.19941400 | -0.09458900 | 2.51673500 |
| C | -3.50381400 | -0.86719900 | 3.36821200 |
| H | -5.17229100 | -0.38062100 | 2.05330500 |
| H | -4.24490200 | 1.01651200 | 2.59659700 |
| H | -1.58732600 | -1.08450200 | 4.38446000 |
| H | -2.04239200 | 0.58309700 | 4.04012800 |
| H | -4.09048800 | -0.79163500 | 4.29269900 |
| H | -3.51887900 | -1.92678800 | 3.07337300 |
| F | -2.37056300 | 6.30149100 | -1.07618500 |
| F | 7.67696400 | -0.67658900 | 0.44098400 |
| F | -3.35599200 | -5.41831400 | -1.86934400 |

**Ar=3,5-diF-Ph, R=Cy**

Zero-point correction= 0.440580 (Hartree/Particle)
Thermal correction to Energy= 0.470740
Thermal correction to Enthalpy= 0.471684
Thermal correction to Gibbs Free Energy= 0.375527
Sum of electronic and zero-point Energies= -1771.614472
Sum of electronic and thermal Energies= -1771.584313
Sum of electronic and thermal Enthalpies= -1771.583369
Sum of electronic and thermal Free Energies= -1771.679526
Single-point electronic energy (M06) = - -1771.48262919 C
0.06000000 1.30042300 -0.34090100

| | | | |
|---|---|---|---|
| C | -0.17921300 | -1.02313600 | -0.49357400 |
| C | 1.43989100 | 1.17593000 | -0.23243500 |
| C | 1.19562700 | -1.19632600 | -0.37228200 |
| C | 2.05107100 | -0.09118400 | -0.21098000 |
| H | 2.05205800 | 2.07017700 | -0.19990800 |
| H | 1.61869400 | -2.18562500 | -0.50948100 |
| N | -0.77463100 | 0.20911300 | -0.38729000 |
| C | -0.58865900 | 2.63080900 | -0.43493700 |
| C | 0.00221000 | 3.77730500 | 0.12626300 |
| C | -1.81719900 | 2.75742500 | -1.10612800 |
| C | -0.63189900 | 5.00439600 | -0.00936500 |
| H | 0.92725100 | 3.72762900 | 0.68865400 |
| C | -2.40811800 | 4.00817100 | -1.21365200 |
| H | -2.29345700 | 1.89229000 | -1.54952100 |
| C | -1.84195700 | 5.15914200 | -0.67641900 |
| C | -1.06423800 | -2.17029000 | -0.81539000 |
| C | -2.21054800 | -1.96516800 | -1.60151000 |
| C | -0.75931000 | -3.47224700 | -0.38064300 |
| C | -3.00846300 | -3.04998500 | -1.93595300 |
| H | -2.46663600 | -0.97417500 | -1.95436500 |
| C | -1.59264600 | -4.52244600 | -0.74126400 |
| H | 0.09733500 | -3.67642700 | 0.25134100 |
| C | -2.72979200 | -4.34832900 | -1.52160900 |
| C | 3.51456400 | -0.25442300 | -0.10053700 |
| C | 4.05835800 | -1.39802700 | 0.51309100 |
| C | 4.39278400 | 0.72220200 | -0.60610800 |
| C | 5.43639700 | -1.53625000 | 0.60360300 |

| | | | |
|---|---|---|---|
| H | 3.42507600 | -2.16264300 | 0.94784500 |
| C | 5.76261600 | 0.53540200 | -0.48876600 |
| H | 4.02856000 | 1.60391600 | -1.12039800 |
| C | 6.32399800 | -0.58578700 | 0.11256500 |
| C | -1.93023400 | 0.31809100 | 1.41407200 |
| C | -3.35142000 | -0.07824300 | 1.13727600 |
| C | -1.21291100 | -0.52411900 | 2.42842900 |
| H | -1.76695300 | 1.38993100 | 1.50732400 |
| C | -4.15304600 | -0.06448700 | 2.46624000 |
| H | -3.38505500 | -1.09239100 | 0.72144500 |
| H | -3.81324000 | 0.59217300 | 0.40439100 |
| C | -2.01295700 | -0.52557500 | 3.75895000 |
| H | -1.13723000 | -1.56030900 | 2.06975100 |
| H | -0.19261600 | -0.16111200 | 2.59885400 |
| C | -3.47444300 | -0.94105000 | 3.53022900 |
| H | -5.17897300 | -0.40723100 | 2.28023300 |
| H | -4.22674100 | 0.96821000 | 2.83520500 |
| H | -1.52753300 | -1.19757100 | 4.47849900 |
| H | -1.98376600 | 0.48153600 | 4.19773700 |
| H | -4.03120300 | -0.88769600 | 4.47436100 |
| H | -3.50579700 | -1.99190800 | 3.20720600 |
| H | -2.32105400 | 6.12627700 | -0.76834100 |
| H | 7.39667000 | -0.71187700 | 0.19361300 |
| H | -3.36780900 | -5.18123400 | -1.79105900 |
| F | -3.58009400 | 4.11804500 | -1.87034100 |
| F | -0.05839600 | 6.09327700 | 0.54075800 |
| F | 6.58870400 | 1.47512600 | -0.98952200 |
| F | 5.93835600 | -2.63338700 | 1.20421800 |
| F | -1.29465300 | -5.76345200 | -0.30755200 |
| F | -4.09924300 | -2.84284100 | -2.69999800 |

**Ar=Ph, R=iPr**

Zero-point correction= 0.423278 (Hartree/Particle)
Thermal correction to Energy= 0.446653
Thermal correction to Enthalpy= 0.447597
Thermal correction to Gibbs Free Energy= 0.368156
Sum of electronic and zero-point Energies= -1059.498069
Sum of electronic and thermal Energies= -1059.474695
Sum of electronic and thermal Enthalpies= -1059.473750
Sum of electronic and thermal Free Energies= -1059.553192
Single-point electronic energy (M06) = -1059.36246244

| | | | |
|---|---|---|---|
| C | -2.05422100 | 0.19140600 | 1.74943900 |
| H | -1.98802600 | 1.27602300 | 1.78816500 |
| C | -0.27864400 | 1.24122300 | -0.15534800 |
| C | -0.37025900 | -1.10155300 | -0.20962100 |
| C | 1.11108000 | 1.20836400 | -0.14580400 |
| C | 1.01824900 | -1.17637700 | -0.18995500 |
| C | 1.80933000 | -0.01364800 | -0.12711400 |
| H | 1.66049700 | 2.14237900 | -0.19036000 |
| H | 1.49582100 | -2.14063100 | -0.32892500 |
| N | -1.04017700 | 0.09462700 | -0.09547700 |
| C | -1.01922100 | 2.52309000 | -0.24592900 |
| C | -0.48764100 | 3.72525100 | 0.25587700 |
| C | -2.28634100 | 2.56319300 | -0.85573600 |
| C | -1.18938300 | 4.92343600 | 0.13763200 |
| H | 0.47134400 | 3.71880900 | 0.76606800 |
| C | -2.98662100 | 3.76167600 | -0.97391800 |
| H | -2.70395600 | 1.64136700 | -1.24633900 |
| C | -2.44175100 | 4.94897100 | -0.47975900 |
| H | -0.76077300 | 5.83811600 | 0.53907000 |
| H | -3.95984000 | 3.76988900 | -1.45825500 |
| C | -1.19551300 | -2.31834100 | -0.40924900 |
| C | -2.40194900 | -2.24546400 | -1.12763100 |
| C | -0.78807700 | -3.57346600 | 0.07722200 |
| C | -3.16761000 | -3.38625800 | -1.35798200 |
| H | -2.72252000 | -1.28160600 | -1.50854300 |
| C | -1.55550400 | -4.71441800 | -0.15163300 |
| H | 0.12633200 | -3.65233900 | 0.65876200 |
| C | -2.74868100 | -4.62716400 | -0.87156000 |
| H | -4.09231900 | -3.30783100 | -1.92412400 |
| H | -1.22450400 | -5.67236300 | 0.24113500 |
| C | 3.28464000 | -0.07843500 | -0.10968000 |
| C | 3.94973800 | -1.15346200 | 0.51042000 |
| C | 4.07283000 | 0.92357000 | -0.70722100 |
| C | 5.34099800 | -1.22432700 | 0.53154700 |
| H | 3.36761400 | -1.92632500 | 1.00453000 |
| C | 5.46379300 | 0.85340100 | -0.68406100 |
| H | 3.59085600 | 1.74966300 | -1.22207000 |
| C | 6.10696200 | -0.22068500 | -0.06461900 |
| H | 5.82830600 | -2.06196000 | 1.02403700 |
| H | 6.04799100 | 1.63602500 | -1.16135700 |
| C | -3.44309200 | -0.33230000 | 1.54273900 |
| H | -3.45074400 | -1.40927400 | 1.35030900 |
| H | -4.05288200 | -0.15627600 | 2.44570800 |
| H | -3.94141900 | 0.17351100 | 0.71001300 |
| C | -1.15690600 | -0.52390600 | 2.71299300 |
| H | -1.53552700 | -0.41686900 | 3.74341800 |
| H | -1.10894800 | -1.59837900 | 2.50108300 |
| H | -0.13909000 | -0.11928200 | 2.69684500 |
| H | 7.19204000 | -0.27468600 | -0.04732000 |
| H | -3.34726800 | -5.51647300 | -1.04958800 |
| H | -2.98896300 | 5.88344500 | -0.57021100 |

**Ar=4-Me-Ph, R=iPr**

Zero-point correction= 0.505786 (Hartree/Particle)
Thermal correction to Energy= 0.534897
Thermal correction to Enthalpy= 0.535841
Thermal correction to Gibbs Free Energy= 0.441459
Sum of electronic and zero-point Energies= -1177.370013
Sum of electronic and thermal Energies= -1177.340901
Sum of electronic and thermal Enthalpies= -1177.339957
Sum of electronic and thermal Free Energies= -1177.434339
Single-point electronic energy (M06) = -1177.24747336

| | | | |
|---|---|---|---|
| C | -2.04144600 | 0.15557100 | 1.86349400 |
| H | -2.00105900 | 1.24190800 | 1.88754100 |
| C | -0.34847300 | 1.22629700 | -0.09746200 |
| C | -0.37188900 | -1.11927600 | -0.11437800 |
| C | 1.04145200 | 1.23358200 | -0.11931400 |
| C | 1.01839700 | -1.15290800 | -0.12768000 |
| C | 1.77651100 | 0.03313500 | -0.09961200 |
| H | 1.56181000 | 2.18245800 | -0.19090300 |
| H | 1.51994200 | -2.10516000 | -0.26535300 |
| N | -1.07454200 | 0.05861100 | -0.00089200 |
| C | -1.12844600 | 2.48328400 | -0.18985800 |
| C | -0.62311000 | 3.71294300 | 0.26860200 |
| C | -2.41238400 | 2.48117000 | -0.76303100 |
| C | -1.36358100 | 4.88551800 | 0.14489800 |
| H | 0.35154100 | 3.75187900 | 0.74692800 |
| C | -3.14696200 | 3.65730000 | -0.88431900 |
| H | -2.81747100 | 1.54355800 | -1.12868100 |
| C | -2.64051300 | 4.88333400 | -0.43242700 |
| H | -0.94495800 | 5.82004400 | 0.51275300 |
| H | -4.13210200 | 3.62472300 | -1.34542600 |
| C | -1.16419800 | -2.36232200 | -0.27417100 |
| C | -2.39323500 | -2.34184800 | -0.95672800 |
| C | -0.71168900 | -3.59895700 | 0.21564000 |
| C | -3.12793800 | -3.50790300 | -1.14640000 |
| H | -2.75968800 | -1.39563900 | -1.34085100 |
| C | -1.45295100 | -4.76331800 | 0.02413800 |
| H | 0.21830300 | -3.64767400 | 0.77557900 |
| C | -2.67257600 | -4.74362800 | -0.66353900 |
| H | -4.07280800 | -3.46077900 | -1.68431300 |
| H | -1.08106600 | -5.70361200 | 0.42557400 |
| C | 3.25230300 | 0.01312700 | -0.11737900 |
| C | 3.97038000 | -1.03926600 | 0.48057600 |
| C | 3.99981600 | 1.03479900 | -0.73203500 |
| C | 5.36199000 | -1.06630100 | 0.46350100 |
| H | 3.43025400 | -1.83504400 | 0.98597100 |
| C | 5.39125200 | 1.00341300 | -0.74393400 |
| H | 3.48591400 | 1.84690700 | -1.23836500 |
| C | 6.10302600 | -0.04444800 | -0.14447000 |
| H | 5.88387200 | -1.89406700 | 0.93942800 |

| | | | |
|---|---|---|---|
| H | 5.93664000 | 1.80365900 | -1.23998700 |
| C | -3.42276300 | -0.40333900 | 1.70040900 |
| H | -3.40950300 | -1.48257800 | 1.52115500 |
| H | -4.01308800 | -0.23042600 | 2.61690900 |
| H | -3.95447400 | 0.07962200 | 0.87472100 |
| C | -1.10536600 | -0.52446600 | 2.81606400 |
| H | -1.46341900 | -0.41347300 | 3.85348000 |
| H | -1.03487800 | -1.60006100 | 2.61642400 |
| H | -0.09864300 | -0.09503700 | 2.77152100 |
| C | -3.46298200 | -6.00953100 | -0.89647300 |
| H | -4.53961800 | -5.83791500 | -0.78444400 |
| H | -3.30320700 | -6.39870100 | -1.91117200 |
| H | -3.17202500 | -6.79865700 | -0.19530200 |
| C | -3.45382400 | 6.15197000 | -0.53458600 |
| H | -4.14721800 | 6.11631600 | -1.38174400 |
| H | -4.05551600 | 6.31520400 | 0.37007500 |
| H | -2.81276000 | 7.03153800 | -0.65879400 |
| C | 7.61328600 | -0.05918400 | -0.13191700 |
| H | 8.00494900 | -1.08218600 | -0.14469400 |
| H | 8.02658400 | 0.47194600 | -0.99617300 |
| H | 8.01096600 | 0.42848500 | 0.76872800 |

**Ar=4-MeO-Ph, R=iPr**

Zero-point correction= 0.521401 (Hartree/Particle)
Thermal correction to Energy= 0.552736
Thermal correction to Enthalpy= 0.553680
Thermal correction to Gibbs Free Energy= 0.455001
Sum of electronic and zero-point Energies= -1402.968304
Sum of electronic and thermal Energies= -1402.936969
Sum of electronic and thermal Enthalpies= -1402.936025
Sum of electronic and thermal Free Energies= -1403.034704
Single-point electronic energy (M06) = -1402.84753984

| | | | |
|---|---|---|---|
| C | 1.90931900 | 0.03734400 | 2.02953200 |
| H | 2.02602400 | -1.04366900 | 2.03919000 |
| C | 0.46964600 | -1.21117500 | -0.01310800 |
| C | 0.19897500 | 1.12060400 | -0.01056700 |
| C | -0.90631200 | -1.39096600 | -0.09796500 |
| C | -1.18215500 | 0.97999300 | -0.08842700 |
| C | -1.78662800 | -0.29217700 | -0.10238900 |
| H | -1.30038900 | -2.39609000 | -0.20212400 |
| H | -1.79272800 | 1.86302600 | -0.24669800 |
| N | 1.03867500 | 0.03757100 | 0.13070200 |
| C | 1.40394600 | -2.35809600 | -0.08190900 |
| C | 1.03499900 | -3.65445200 | 0.33208300 |
| C | 2.70432100 | -2.18724200 | -0.58067800 |
| C | 1.91433300 | -4.72252000 | 0.23630900 |
| H | 0.05137900 | -3.82487800 | 0.76010300 |
| C | 3.59994900 | -3.25186100 | -0.68389000 |
| H | 3.00916700 | -1.19788800 | -0.90501000 |
| C | 3.20641600 | -4.53199400 | -0.27648400 |
| H | 1.62843800 | -5.71703300 | 0.56479000 |
| H | 4.59103500 | -3.07370800 | -1.08612200 |
| C | 0.83662100 | 2.45279700 | -0.12852000 |
| C | 2.08037500 | 2.59517500 | -0.76018900 |
| C | 0.21274800 | 3.62362900 | 0.34686200 |
| C | 2.68392400 | 3.84212800 | -0.92470600 |
| H | 2.57606700 | 1.70669500 | -1.13702600 |
| C | 0.80100600 | 4.87081300 | 0.19355800 |
| H | -0.73967000 | 3.55186600 | 0.86474600 |
| C | 2.04322300 | 4.99197200 | -0.44677300 |
| H | 3.64165800 | 3.90567700 | -1.42909500 |
| H | 0.32210300 | 5.76928000 | 0.57050400 |
| C | -3.25027700 | -0.45617500 | -0.18669200 |
| C | -4.12092500 | 0.48328300 | 0.38840900 |
| C | -3.83908600 | -1.55669300 | -0.84497800 |
| C | -5.50819000 | 0.34829700 | 0.31815100 |
| H | -3.70902400 | 1.33043400 | 0.92961400 |
| C | -5.21521300 | -1.70614800 | -0.92195800 |
| H | -3.20588400 | -2.29332100 | -1.33108300 |
| C | -6.06543700 | -0.75358900 | -0.33990500 |
| H | -6.13723000 | 1.09671400 | 0.78697700 |
| H | -5.66017400 | -2.54993400 | -1.44047400 |
| C | 3.20376200 | 0.79095200 | 1.95581000 |
| H | 3.04564100 | 1.86031700 | 1.78596800 |
| H | 3.75901000 | 0.68817800 | 2.90424600 |
| H | 3.84685000 | 0.40472900 | 1.15860200 |
| C | 0.83835400 | 0.55551600 | 2.94137200 |
| H | 1.15302000 | 0.47246800 | 3.99528600 |
| H | 0.62542700 | 1.61448500 | 2.75392700 |
| H | -0.09300700 | -0.01081300 | 2.83328100 |
| O | -7.40431100 | -0.99114400 | -0.46963900 |
| O | 3.99468700 | -5.64566900 | -0.32950300 |
| O | 2.53814700 | 6.26060700 | -0.54863300 |
| C | 3.79316900 | 6.44151300 | -1.18374300 |
| H | 3.76861000 | 6.10959800 | -2.23028300 |
| H | 3.99377200 | 7.51407100 | -1.15108100 |
| H | 4.59434400 | 5.90685100 | -0.65615800 |
| C | 5.31337500 | -5.51023500 | -0.83342000 |
| H | 5.75672500 | -6.50660100 | -0.78445600 |
| H | 5.31471200 | -5.16429300 | -1.87568600 |
| H | 5.91006300 | -4.81792300 | -0.22450500 |
| C | -8.30714200 | -0.05066100 | 0.08778800 |
| H | -8.18366800 | 0.94363600 | -0.36199100 |
| H | -9.30757900 | -0.42580800 | -0.13602300 |
| H | -8.18617800 | 0.03038800 | 1.17641600 |

**Ar=4-CF3-Ph, R=iPr**

Zero-point correction= 0.437316 (Hartree/Particle)
Thermal correction to Energy= 0.471807
Thermal correction to Enthalpy= 0.472751
Thermal correction to Gibbs Free Energy= 0.363474
Sum of electronic and zero-point Energies= -2070.597595
Sum of electronic and thermal Energies= -2070.563103
Sum of electronic and thermal Enthalpies= -2070.562159
Sum of electronic and thermal Free Energies= -2070.671437
Single-point electronic energy (M06) = -2070.46969683

| | | | |
|---|---|---|---|
| C | 2.10337300 | -0.07664300 | 2.04941500 |
| H | 2.12672300 | -1.16355800 | 2.03911700 |
| C | 0.45811700 | -1.19942400 | 0.04071500 |
| C | 0.36348400 | 1.14039300 | 0.06036600 |
| C | -0.92944200 | -1.27768000 | 0.00139100 |
| C | -1.02677300 | 1.10770900 | 0.03468400 |
| C | -1.72268300 | -0.11575900 | 0.02765300 |
| H | -1.40129400 | -2.24972300 | -0.08893700 |
| H | -1.57387000 | 2.03650700 | -0.08784800 |
| N | 1.12351700 | -0.00033900 | 0.15351800 |
| C | 1.29969700 | -2.41549100 | -0.06204400 |
| C | 0.84569200 | -3.67278900 | 0.37781300 |
| C | 2.58719700 | -2.33581700 | -0.62272600 |
| C | 1.64004500 | -4.80696000 | 0.24981900 |
| H | -0.12952200 | -3.76338600 | 0.84625000 |
| C | 3.38471300 | -3.46811500 | -0.75225800 |
| H | 2.94624900 | -1.37361900 | -0.97031500 |
| C | 2.91386000 | -4.71005700 | -0.31808600 |
| H | 1.27331400 | -5.76871400 | 0.59393800 |
| H | 4.36910200 | -3.39199400 | -1.20229000 |
| C | 1.09325000 | 2.42459800 | -0.07388400 |
| C | 2.31528100 | 2.47403700 | -0.76808000 |
| C | 0.57711900 | 3.62384600 | 0.44756200 |
| C | 2.99106800 | 3.67641800 | -0.94214000 |
| H | 2.71946700 | 1.55627900 | -1.18065100 |
| C | 1.25247600 | 4.82927000 | 0.27962700 |
| H | -0.35304000 | 3.61155700 | 1.00789900 |
| C | 2.46206700 | 4.86055500 | -0.41814800 |
| H | 3.92374400 | 3.70162900 | -1.49674300 |
| H | 0.84163600 | 5.74543100 | 0.69056700 |
| C | -3.19665800 | -0.16999500 | -0.02120500 |
| C | -3.97621900 | 0.82695300 | 0.59579800 |
| C | -3.87119400 | -1.21480800 | -0.68193000 |
| C | -5.36570900 | 0.78610500 | 0.55236000 |
| H | -3.48743400 | 1.62744500 | 1.14277500 |
| C | -5.25982400 | -1.26080700 | -0.72608000 |

| | | | |
|---|---|---|---|
| H | -3.30240800 | -1.98568100 | -1.19264500 |
| C | -6.01539800 | -0.25956500 | -0.10865100 |
| H | -5.94792100 | 1.55668600 | 1.04699000 |
| H | -5.75989200 | -2.07323500 | -1.24332200 |
| C | 3.44278800 | 0.57459700 | 1.89634100 |
| H | 3.35955300 | 1.65529000 | 1.74788100 |
| H | 4.04377600 | 0.41604800 | 2.80796800 |
| H | 4.00423600 | 0.14851500 | 1.05941600 |
| C | 1.11448100 | 0.52289800 | 3.00004900 |
| H | 1.46693700 | 0.40944400 | 4.03875900 |
| H | 0.98179900 | 1.59694200 | 2.82551100 |
| H | 0.13708000 | 0.03289600 | 2.93429400 |
| C | 3.22673700 | 6.14768500 | -0.55704300 |
| C | 3.79125800 | -5.92828900 | -0.39798100 |
| F | 2.41748600 | 7.22780900 | -0.48614500 |
| F | 4.15462700 | 6.28751600 | 0.42039500 |
| F | 3.88993300 | 6.21192600 | -1.73341800 |
| F | 4.71646600 | -5.82290800 | -1.37713700 |
| F | 3.07260900 | -7.04906300 | -0.63509700 |
| F | 4.46561700 | -6.13670100 | 0.75849500 |
| C | -7.51496000 | -0.27813900 | -0.20790700 |
| F | -7.95277800 | 0.35850500 | -1.32054000 |
| F | -8.09839200 | 0.33429700 | 0.84694100 |
| F | -7.99955600 | -1.53924000 | -0.26525200 |

**Ar=4-F-Ph, R=iPr**

Zero-point correction= 0.398534 (Hartree/Particle)
Thermal correction to Energy= 0.424468
Thermal correction to Enthalpy= 0.425412
Thermal correction to Gibbs Free Energy= 0.339779
Sum of electronic and zero-point Energies= -1357.222748
Sum of electronic and thermal Energies= -1357.196813
Sum of electronic and thermal Enthalpies= -1357.195869
Sum of electronic and thermal Free Energies= -1357.281502
Single-point electronic energy (M06) = -1357.08654296

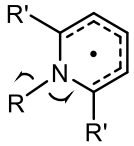
| | | | |
|---|---|---|---|
| C | -2.04427600 | 0.15561100 | 1.85972500 |
| H | -2.01050500 | 1.24222500 | 1.88243500 |
| C | -0.34421600 | 1.22769700 | -0.09610700 |
| C | -0.37586500 | -1.11710500 | -0.12051400 |
| C | 1.04556600 | 1.23079000 | -0.11437600 |
| C | 1.01404200 | -1.15614600 | -0.13056100 |
| C | 1.77568300 | 0.02744600 | -0.09625300 |
| H | 1.56987500 | 2.17787100 | -0.18259300 |
| H | 1.51347800 | -2.10900800 | -0.27252500 |
| N | -1.07517900 | 0.06262900 | -0.00393400 |
| C | -1.12012000 | 2.48750200 | -0.18799800 |
| C | -0.61177600 | 3.71164200 | 0.28474200 |
| C | -2.40111600 | 2.48598500 | -0.77075100 |
| C | -1.34067500 | 4.89275200 | 0.16754900 |
| H | 0.35696900 | 3.74157800 | 0.77426800 |
| C | -3.14223800 | 3.65799600 | -0.89484400 |
| H | -2.80413200 | 1.54890800 | -1.13861800 |
| C | -2.59779800 | 4.84781500 | -0.42452900 |
| H | -0.95532400 | 5.83703900 | 0.53811800 |
| H | -4.12589900 | 3.66308000 | -1.35337200 |
| C | -1.17389000 | -2.35582600 | -0.28730100 |
| C | -2.39794400 | -2.32252400 | -0.97940600 |
| C | -0.72555600 | -3.59540500 | 0.20359200 |
| C | -3.14596000 | -3.47884900 | -1.18326200 |
| H | -2.75289000 | -1.37287600 | -1.36442900 |
| C | -1.46226100 | -4.76181400 | 0.00881400 |
| H | 0.20238700 | -3.64751900 | 0.76545700 |
| C | -2.66435900 | -4.68478200 | -0.68493200 |
| H | -4.08614700 | -3.46030800 | -1.72506700 |
| H | -1.12485000 | -5.71858800 | 0.39376200 |
| C | 3.25171300 | 0.00154100 | -0.11195600 |
| C | 3.96088000 | -1.04580900 | 0.50740900 |
| C | 3.99988600 | 1.01447200 | -0.74272000 |
| C | 5.35289300 | -1.08763200 | 0.50016600 |
| H | 3.41414900 | -1.82703700 | 1.02698700 |
| C | 5.39178600 | 0.98929200 | -0.75612000 |
| H | 3.48660600 | 1.82038500 | -1.25831100 |
| C | 6.04978100 | -0.06504400 | -0.13255200 |
| H | 5.89967700 | -1.88972900 | 0.98523200 |
| H | 5.96860600 | 1.76371500 | -1.25126400 |
| C | -3.42235400 | -0.41149100 | 1.69807600 |
| H | -3.40448900 | -1.49266900 | 1.53134200 |
| H | -4.01510200 | -0.23153600 | 2.61125900 |
| H | -3.95545700 | 0.06020200 | 0.86676300 |
| C | -1.10369600 | -0.51659500 | 2.81320100 |
| H | -1.46269300 | -0.40465500 | 3.84990600 |
| H | -1.02744300 | -1.59247600 | 2.61723100 |
| H | -0.09955200 | -0.08132600 | 2.76798600 |
| F | 7.39929300 | -0.09575800 | -0.14194800 |
| F | -3.31054800 | 5.98816100 | -0.53922800 |
| F | -3.38538700 | -5.80960200 | -0.87566500 |

**Ar=3,5-diF-Ph, R=iPr**

Zero-point correction= 0.373428 (Hartree/Particle)
Thermal correction to Energy= 0.402057
Thermal correction to Enthalpy= 0.403002
Thermal correction to Gibbs Free Energy= 0.311003
Sum of electronic and zero-point Energies= -1654.946057
Sum of electronic and thermal Energies= -1654.917428
Sum of electronic and thermal Enthalpies= -1654.916483
Sum of electronic and thermal Free Energies= -1655.008482
Single-point electronic energy (M06) = -1654.80782651

| | | | |
|---|---|---|---|
| C | -2.03047500 | 0.12172100 | 1.97544400 |
| H | -1.99651000 | 1.20811800 | 2.00049000 |
| C | -0.37313200 | 1.22195800 | -0.02729100 |
| C | -0.41075100 | -1.11737000 | -0.09529600 |
| C | 1.01554500 | 1.22512600 | -0.08312900 |
| C | 0.97819500 | -1.16170800 | -0.14132900 |
| C | 1.74155100 | 0.02010900 | -0.10907100 |
| H | 1.53987900 | 2.17207800 | -0.14470100 |
| H | 1.47080100 | -2.11366300 | -0.30778800 |
| N | -1.10365100 | 0.05910500 | 0.05549800 |
| C | -1.14748400 | 2.48607600 | -0.07581500 |
| C | -0.60510100 | 3.69785900 | 0.38870300 |
| C | -2.44902000 | 2.48245700 | -0.60663200 |
| C | -1.35923900 | 4.85953800 | 0.29770500 |
| H | 0.37744800 | 3.74860100 | 0.84319000 |
| C | -3.15958900 | 3.67220200 | -0.67504700 |
| H | -2.89049600 | 1.56521200 | -0.97508300 |
| C | -2.64466300 | 4.88548200 | -0.23154300 |
| C | -1.21530700 | -2.35204000 | -0.26916300 |
| C | -2.45725000 | -2.28779100 | -0.92270400 |
| C | -0.74240100 | -3.59863800 | 0.17718000 |
| C | -3.18327700 | -3.45382300 | -1.11813800 |
| H | -2.84306600 | -1.34186400 | -1.28130500 |
| C | -1.50911900 | -4.73511700 | -0.04260000 |
| H | 0.19591000 | -3.69433300 | 0.71141400 |
| C | -2.73892200 | -4.70042700 | -0.68963400 |
| C | 3.21647000 | -0.00703300 | -0.16877600 |
| C | 3.93065600 | -1.08642500 | 0.38404500 |
| C | 3.93759100 | 1.03822500 | -0.77575400 |
| C | 5.31682000 | -1.09638200 | 0.31699000 |
| H | 3.42506100 | -1.89930700 | 0.89222900 |
| C | 5.32326800 | 0.98007400 | -0.81404400 |
| H | 3.43792200 | 1.87528200 | -1.24920100 |
| C | 6.05100800 | -0.07568900 | -0.27580800 |
| C | -3.40702500 | -0.45226800 | 1.84204300 |
| H | -3.38626500 | -1.53117100 | 1.66204700 |
| H | -3.97335100 | -0.28820500 | 2.77471900 |
| H | -3.96768000 | 0.02656000 | 1.03372000 |
| C | -1.05068600 | -0.56014000 | 2.87901600 |
| H | -1.37329300 | -0.46821200 | 3.92946500 |
| H | -0.97575700 | -1.63219100 | 2.66274700 |
| H | -0.05192900 | -0.11655500 | 2.80673900 |
| H | -3.32284300 | -5.59859400 | -0.84990500 |
| H | 7.13302500 | -0.10127100 | -0.31665100 |
| H | -3.21706700 | 5.80318300 | -0.29064600 |

| | | | |
|---|---|---|---|
| F | -1.04893900 | -5.92212600 | 0.39995600 |
| F | -4.36846700 | -3.38198700 | -1.75570300 |
| F | -4.40182900 | 3.65703800 | -1.19768000 |
| F | -0.82950300 | 6.01171800 | 0.75441900 |
| F | 5.99644100 | 1.98450700 | -1.40907900 |
| F | 5.98316100 | -2.13395500 | 0.86074600 |




**R'=H, R=Et**

Zero-point correction= 0.151394 (Hartree/Particle)
Thermal correction to Energy= 0.159446
Thermal correction to Enthalpy= 0.160390
Thermal correction to Gibbs Free Energy= 0.117531
Sum of electronic and zero-point Energies= -327.273418
Sum of electronic and thermal Energies= -327.265366
Sum of electronic and thermal Enthalpies= -327.264422
Sum of electronic and thermal Free Energies= -327.307281
Single-point electronic energy (M06) = -327.24944

| | | | |
|---|---|---|---|
| C | 2.26418800 | 0.00000800 | -0.37227400 |
| H | 2.57175800 | -0.91046500 | -0.88153300 |
| C | -0.33894800 | -1.15604000 | -0.57313000 |
| C | -0.33895600 | 1.15605000 | -0.57311600 |
| C | -1.49236700 | -1.19804100 | 0.19510800 |
| C | -1.49237600 | 1.19803400 | 0.19512200 |
| C | -2.09356900 | -0.00000800 | 0.60206400 |
| H | -1.92906600 | -2.15960900 | 0.45175600 |
| H | -1.92908300 | 2.15959600 | 0.45178000 |
| N | 0.27326200 | 0.00001000 | -0.95482900 |
| C | 2.27326000 | -0.00000900 | 1.12296400 |
| H | 3.29670300 | -0.00005400 | 1.53302100 |
| H | 1.76617900 | 0.88665300 | 1.52422600 |
| H | 1.76611100 | -0.88664300 | 1.52420400 |
| H | -2.99592200 | -0.00001500 | 1.20539200 |
| H | 2.57176300 | 0.91048800 | -0.88151500 |
| H | 0.14067600 | -2.07205600 | -0.91198800 |
| H | 0.14066200 | 2.07207400 | -0.91196000 |

**R'=Me, R=Et**

Zero-point correction= 0.207315 (Hartree/Particle)
Thermal correction to Energy= 0.218477
Thermal correction to Enthalpy= 0.219421
Thermal correction to Gibbs Free Energy= 0.169921
Sum of electronic and zero-point Energies= -405.856036
Sum of electronic and thermal Energies= -405.844874
Sum of electronic and thermal Enthalpies= -405.843930
Sum of electronic and thermal Free Energies= -405.893430
Single-point electronic energy (M06) = -405.84598

| | | | |
|---|---|---|---|
| C | -0.20456400 | 2.14411600 | 0.00945300 |
| H | 0.67039000 | 2.59144500 | -0.45295000 |
| C | 1.20928000 | -0.27793000 | -0.36769000 |
| C | -1.12751200 | -0.50374000 | -0.37361000 |
| C | 1.34323300 | -1.44104200 | 0.38146000 |
| C | -1.04027700 | -1.67169600 | 0.37479800 |
| C | 0.20808200 | -2.15284500 | 0.78204500 |
| H | 2.33886500 | -1.80850000 | 0.61666400 |
| H | -1.94837800 | -2.22318900 | 0.60455200 |
| N | -0.01856500 | 0.23329600 | -0.70846600 |
| C | -0.21795000 | 2.04361400 | 1.50345900 |
| H | -0.30469300 | 3.03235900 | 1.98323400 |
| H | -1.06192100 | 1.43838100 | 1.85715300 |
| H | 0.70216800 | 1.58110800 | 1.88200200 |
| H | 0.29480400 | -3.06482900 | 1.36462400 |
| C | -2.45308500 | 0.01612000 | -0.86725000 |
| H | -2.79343900 | 0.88205300 | -0.28395200 |
| H | -2.37659600 | 0.34060000 | -1.91087200 |
| H | -3.22750200 | -0.75368300 | -0.79598700 |
| C | 2.41364100 | 0.48565900 | -0.85519600 |
| H | 2.58951200 | 1.39173800 | -0.26026900 |
| H | 3.31785800 | -0.12765600 | -0.79506200 |
| H | 2.27457200 | 0.80384700 | -1.89417100 |
| H | -1.13077600 | 2.42972000 | -0.48051500 |

**R'=Ph, R=Et**

Zero-point correction= 0.313664 (Hartree/Particle)
Thermal correction to Energy= 0.330896
Thermal correction to Enthalpy= 0.331841
Thermal correction to Gibbs Free Energy= 0.266468
Sum of electronic and zero-point Energies= -789.231777
Sum of electronic and thermal Energies= -789.214545
Sum of electronic and thermal Enthalpies= -789.213600
Sum of electronic and thermal Free Energies= -789.278973
Single-point electronic energy (M06) = -789.12222

| | | | |
|---|---|---|---|
| C | -0.00005200 | -0.54782400 | 1.84442300 |
| H | -0.91347000 | -1.13176900 | 1.79460300 |
| C | -1.17741400 | 0.81645100 | -0.36708300 |
| C | 1.17746300 | 0.81644700 | -0.36704300 |
| C | -1.19913100 | 2.17774700 | -0.67439400 |
| C | 1.19918500 | 2.17774800 | -0.67435100 |
| C | 0.00003100 | 2.87911600 | -0.81244700 |
| H | -2.14557400 | 2.67064200 | -0.87162300 |
| H | 2.14563100 | 2.67064600 | -0.87155400 |
| N | 0.00001900 | 0.14599000 | -0.14692300 |
| C | -2.42259900 | 0.01677700 | -0.28688800 |
| C | -3.65446300 | 0.60043400 | 0.06040700 |
| C | -2.39790000 | -1.36179400 | -0.56545200 |
| C | -4.81936500 | -0.16237200 | 0.11244900 |
| H | -3.69861100 | 1.65497500 | 0.31724300 |
| C | -3.56314800 | -2.12359400 | -0.51320300 |
| H | -1.45220900 | -1.82032100 | -0.83451700 |
| C | -4.78072500 | -1.52821900 | -0.17590700 |
| H | -5.75834700 | 0.30982600 | 0.38962800 |
| H | -3.52147100 | -3.18562000 | -0.74148700 |
| H | -5.68930000 | -2.12286800 | -0.13373300 |
| C | 2.42264800 | 0.01677800 | -0.28682700 |
| C | 2.39793900 | -1.36182000 | -0.56526600 |
| C | 3.65452900 | 0.60046200 | 0.06036400 |
| C | 3.56318900 | -2.12361500 | -0.51300800 |
| H | 1.45223500 | -1.82037300 | -0.83423900 |
| C | 4.81943500 | -0.16233900 | 0.11241300 |
| H | 3.69869000 | 1.65502000 | 0.31712600 |
| C | 4.78078400 | -1.52820900 | -0.17582700 |
| H | 3.52150100 | -3.18566100 | -0.74119400 |
| H | 5.75842900 | 0.30988500 | 0.38950800 |
| H | 5.68936200 | -2.12285300 | -0.13364900 |
| C | -0.00031700 | 0.67835300 | 2.69749900 |
| H | -0.00021700 | 0.42215400 | 3.76996000 |
| H | 0.88820700 | 1.29492900 | 2.51545400 |
| H | -0.88914400 | 1.29450500 | 2.51551100 |
| H | 0.00003700 | 3.93321600 | -1.07243100 |
| H | 0.91358200 | -1.13143600 | 1.79469500 |

**R'=CF3, R=Et**

Zero-point correction= 0.161513 (Hartree/Particle)
Thermal correction to Energy= 0.176318
Thermal correction to Enthalpy= 0.177262
Thermal correction to Gibbs Free Energy= 0.117982
Sum of electronic and zero-point Energies= -1001.337570
Sum of electronic and thermal Energies= -1001.322765
Sum of electronic and thermal Enthalpies= -1001.321821
Sum of electronic and thermal Free Energies= -1001.381100
Single-point electronic energy (M06) = -1001.3175

| | | | |
|---|---|---|---|
| C | -0.00002100 | -2.02666600 | 0.50644500 |
| H | -0.91030600 | -2.37161500 | 0.02996300 |
| C | -1.15137100 | 0.59475000 | -0.04184300 |
| C | 1.15136700 | 0.59476900 | -0.04186100 |
| C | -1.19627900 | 1.81543000 | 0.61764800 |
| C | 1.19626300 | 1.81546000 | 0.61760700 |
| C | -0.00001100 | 2.44194300 | 0.97701700 |
| H | -2.15460500 | 2.28376800 | 0.81244900 |
| H | 2.15458300 | 2.28381500 | 0.81239100 |

| | | | |
|---|---|---|---|
| N | -0.00000100 | -0.07097100 | -0.34168100 |
| C | 0.00007600 | -1.84463400 | 1.98729500 |
| H | -0.00045600 | -2.81962800 | 2.50238800 |
| H | 0.89324500 | -1.30705000 | 2.32500300 |
| H | -0.89255200 | -1.30614200 | 2.32501600 |
| H | -0.00001400 | 3.39752400 | 1.48977400 |
| C | 2.43950400 | -0.08443400 | -0.44385100 |
| C | -2.43951200 | -0.08444600 | -0.44383900 |
| H | 0.91017400 | -2.37167600 | 0.02983400 |
| F | -2.31609100 | -0.77745300 | -1.58762100 |
| F | -3.43585400 | 0.81440100 | -0.60563500 |
| F | -2.86365300 | -0.96058200 | 0.50755900 |
| F | 2.31609100 | -0.77739500 | -1.58765800 |
| F | 3.43586900 | 0.81440000 | -0.60557700 |
| F | 2.86362100 | -0.96061900 | 0.50751700 |

**R'=Cl, R=Et**

Zero-point correction= 0.132320 (Hartree/Particle)
Thermal correction to Energy= 0.142643
Thermal correction to Enthalpy= 0.143587
Thermal correction to Gibbs Free Energy= 0.094328
Sum of electronic and zero-point Energies= -1246.487075
Sum of electronic and thermal Energies= -1246.476752
Sum of electronic and thermal Enthalpies= -1246.475808
Sum of electronic and thermal Free Energies= -1246.525067
Single-point electronic energy (M06) = -1246.4478

| | | | |
|---|---|---|---|
| C | -0.00037400 | -2.09890800 | 0.32476000 |
| H | -0.91149600 | -2.46051700 | -0.14108200 |
| C | -1.13947500 | 0.44727900 | -0.21077100 |
| C | 1.13999300 | 0.44675100 | -0.21049500 |
| C | -1.20284500 | 1.63773400 | 0.49304100 |
| C | 1.20372000 | 1.63716800 | 0.49335800 |
| C | 0.00052700 | 2.24023500 | 0.88016300 |
| H | -2.16336600 | 2.09567700 | 0.70000500 |
| H | 2.16439800 | 2.09466500 | 0.70058300 |
| N | 0.00013500 | -0.21809800 | -0.51407600 |
| C | -0.00195000 | -1.90022800 | 1.80599300 |
| H | -0.00172000 | -2.86740100 | 2.33420500 |
| H | 0.88680700 | -1.35270300 | 2.14220000 |
| H | -0.89211300 | -1.35400400 | 2.14055700 |
| H | 0.00067100 | 3.16535900 | 1.44666100 |
| Cl | 2.63182600 | -0.28862500 | -0.79503600 |
| Cl | -2.63145400 | -0.28753000 | -0.79565600 |
| H | 0.91197700 | -2.45993800 | -0.13911700 |

**R'=tBu, R=Et**

Zero-point correction= 0.377570 (Hartree/Particle)
Thermal correction to Energy= 0.396469
Thermal correction to Enthalpy= 0.397413
Thermal correction to Gibbs Free Energy= 0.332007
Sum of electronic and zero-point Energies= -641.549332
Sum of electronic and thermal Energies= -641.530433
Sum of electronic and thermal Enthalpies= -641.529489
Sum of electronic and thermal Free Energies= -641.594895
Single-point electronic energy (M06) = -641.58933

| | | | |
|---|---|---|---|
| C | 0.00001700 | -1.74111800 | 1.16149400 |
| H | 0.90127200 | -2.26302800 | 0.85567500 |
| C | -1.18229400 | 0.47501000 | 0.00506400 |
| C | 1.18237700 | 0.47494300 | 0.00517800 |
| C | -1.19884400 | 1.71607600 | 0.63213600 |
| C | 1.19894300 | 1.71599800 | 0.63227100 |
| C | 0.00004900 | 2.33092900 | 1.00677900 |
| H | -2.14033900 | 2.23317500 | 0.79079700 |
| H | 2.14045700 | 2.23303700 | 0.79102700 |
| N | 0.00003300 | -0.22215800 | -0.15444900 |
| C | -0.00063400 | -1.16927200 | 2.54708500 |
| H | -0.88755700 | -0.55133400 | 2.72654200 |
| H | -0.00045500 | -1.96788600 | 3.30635200 |
| H | 0.88562600 | -0.55050600 | 2.72698500 |
| H | 0.00005100 | 3.29230700 | 1.51170100 |
| C | 2.47972800 | -0.15160900 | -0.54800200 |
| C | -2.47962700 | -0.15153500 | -0.54815400 |
| C | -3.38229700 | -0.66545200 | 0.60049100 |
| H | -4.32459100 | -1.05824000 | 0.19832700 |
| H | -2.90449600 | -1.46805800 | 1.17114100 |
| H | -3.62800900 | 0.14084800 | 1.30106400 |
| C | -2.18402200 | -1.29935100 | -1.53474800 |
| H | -1.65730100 | -2.13437800 | -1.06895100 |
| H | -3.12803600 | -1.68051100 | -1.94294300 |
| H | -1.56763900 | -0.94976900 | -2.36913100 |
| C | -3.27033800 | 0.92642500 | -1.33256600 |
| H | -4.16114400 | 0.47659000 | -1.78769100 |
| H | -3.61147600 | 1.74574200 | -0.69165900 |
| H | -2.66034500 | 1.35701300 | -2.13431900 |
| C | 2.18421400 | -1.29970700 | -1.53430100 |
| H | 3.12825300 | -1.68073300 | -1.94256200 |
| H | 1.65777800 | -2.13477300 | -1.06825000 |
| H | 1.56760900 | -0.95046200 | -2.36865900 |
| C | 3.38256900 | -0.66510800 | 0.60069100 |
| H | 4.32489300 | -1.05784400 | 0.19854700 |
| H | 3.62820800 | 0.14139000 | 1.30106200 |
| H | 2.90494100 | -1.46765400 | 1.17157400 |
| C | 3.27020900 | 0.92627800 | -1.33275700 |
| H | 3.61116800 | 1.74586100 | -0.69209500 |
| H | 4.16110500 | 0.47649800 | -1.78776000 |
| H | 2.66011400 | 1.35650200 | -2.13462900 |
| H | -0.90062100 | -2.26372700 | 0.85503000 |

**R'=H, R=iPr**

Zero-point correction= 0.179888 (Hartree/Particle)
Thermal correction to Energy= 0.189290
Thermal correction to Enthalpy= 0.190235
Thermal correction to Gibbs Free Energy= 0.144371
Sum of electronic and zero-point Energies= -366.564620
Sum of electronic and thermal Energies= -366.555218
Sum of electronic and thermal Enthalpies= -366.554274
Sum of electronic and thermal Free Energies= -366.600137
Single-point electronic energy (M06) = -366.54903

| | | | |
|---|---|---|---|
| C | 1.86841700 | -0.48637600 | -0.06333900 |
| H | 1.95331400 | -1.38299400 | -0.67686200 |
| C | -0.80770900 | -1.01610500 | -0.80762700 |
| C | -0.45791900 | 1.19602500 | -0.22733800 |
| C | -2.05272100 | -1.02245800 | -0.20149400 |
| C | -1.68853700 | 1.26564600 | 0.40776000 |
| C | -2.51834300 | 0.13759000 | 0.43471400 |
| H | -2.66394800 | -1.92001200 | -0.24728100 |
| H | -2.00685400 | 2.20547300 | 0.85142600 |
| N | 0.02655300 | 0.06519500 | -0.81974400 |
| C | 2.77750100 | 0.63521000 | -0.46632100 |
| H | 2.53002500 | 1.56277400 | 0.06648800 |
| H | 3.82956400 | 0.40753800 | -0.22865600 |
| H | 2.71450600 | 0.82850800 | -1.54266000 |
| C | 1.62727300 | -0.72862500 | 1.39533500 |
| H | 2.53857500 | -1.07873500 | 1.90849900 |
| H | 1.30912700 | 0.19323300 | 1.90073200 |
| H | 0.85119400 | -1.48676000 | 1.55374500 |
| H | -0.42937400 | -1.90185700 | -1.31402000 |
| H | 0.18904500 | 2.06810400 | -0.28335300 |
| H | -3.48882100 | 0.16292200 | 0.92001000 |

**R'=Me, R=iPr**

Zero-point correction= 0.235786 (Hartree/Particle)
Thermal correction to Energy= 0.248383
Thermal correction to Enthalpy= 0.249327
Thermal correction to Gibbs Free Energy= 0.196755
Sum of electronic and zero-point Energies= -445.143130
Sum of electronic and thermal Energies= -445.130533
Sum of electronic and thermal Enthalpies= -445.129589
Sum of electronic and thermal Free Energies= -445.182162
Single-point electronic energy (M06) = -445.14119

| | | | |
|---|---|---|---|
| C | -1.67204300 | 0.66857600 | 0.42994200 |
| H | -1.44036200 | 1.73090600 | 0.44956600 |
| C | 0.99417000 | 1.05653500 | -0.29993300 |
| C | 0.31273700 | -1.18980100 | -0.40569700 |
| C | 2.19780500 | 0.68683100 | 0.28538100 |
| C | 1.50326600 | -1.60009600 | 0.17917600 |

| | | | |
|---|---|---|---|
| C | 2.46248800 | -0.65805000 | 0.56706400 |
| H | 2.94763700 | 1.44998500 | 0.47941200 |
| H | 1.69847600 | -2.66401000 | 0.28851200 |
| N | -0.00070500 | 0.14233200 | -0.57751800 |
| C | -2.85086100 | 0.35640700 | -0.45024100 |
| H | -3.12559200 | -0.70298700 | -0.42163100 |
| H | -3.73764000 | 0.92887100 | -0.13351400 |
| H | -2.64053000 | 0.62551600 | -1.49170300 |
| C | -1.57549300 | 0.01786800 | 1.78080000 |
| H | -2.38890900 | 0.35734900 | 2.44346500 |
| H | -1.65012700 | -1.07407100 | 1.71871600 |
| H | -0.62830200 | 0.26395800 | 2.27412200 |
| H | 3.39794700 | -0.96356700 | 1.02520400 |
| C | -0.68918800 | -2.19406600 | -0.91509900 |
| H | -1.55382600 | -2.29582100 | -0.24771300 |
| H | -1.07397100 | -1.89104700 | -1.89512800 |
| H | -0.23200100 | -3.18395900 | -1.01008300 |
| C | 0.72657900 | 2.49158800 | -0.68394200 |
| H | 0.21151100 | 3.05236600 | 0.10808300 |
| H | 1.66448200 | 3.01793500 | -0.88925700 |
| H | 0.09938500 | 2.53749500 | -1.58013400 |

**R'=Ph, R=iPr**

Zero-point correction= 0.342272 (Hartree/Particle)
Thermal correction to Energy= 0.360822
Thermal correction to Enthalpy= 0.361766
Thermal correction to Gibbs Free Energy= 0.293837
Sum of electronic and zero-point Energies= -828.519544
Sum of electronic and thermal Energies= -828.500995
Sum of electronic and thermal Enthalpies= -828.500050
Sum of electronic and thermal Free Energies= -828.567980
Single-point electronic energy (M06) = -828.41989

| | | | |
|---|---|---|---|
| C | -0.14944500 | -0.49966600 | 1.80185900 |
| H | -1.23681100 | -0.50961700 | 1.81247200 |
| C | -1.24500000 | 0.94387600 | -0.32035000 |
| C | 1.11086100 | 0.94998800 | -0.33311400 |
| C | -1.26985400 | 2.32613200 | -0.49596100 |
| C | 1.12713300 | 2.33410300 | -0.50297800 |
| C | -0.07323700 | 3.04598600 | -0.55614900 |
| H | -2.21748300 | 2.83018000 | -0.65691900 |
| H | 2.07222900 | 2.84156800 | -0.66945400 |
| N | -0.06279700 | 0.25544100 | -0.13717700 |
| C | -2.48639400 | 0.13592800 | -0.34182800 |
| C | -3.72890600 | 0.67555000 | 0.04037200 |
| C | -2.44984800 | -1.20738100 | -0.75969100 |
| C | -4.89002000 | -0.09298100 | -0.00863500 |
| H | -3.78327400 | 1.69783900 | 0.40358400 |
| C | -3.61159600 | -1.97447700 | -0.80874000 |
| H | -1.49732600 | -1.63229400 | -1.05788900 |
| C | -4.83887000 | -1.42184400 | -0.43532200 |
| H | -5.83654500 | 0.34487100 | 0.29791300 |
| H | -3.55972600 | -3.00708400 | -1.14480400 |
| H | -5.74470600 | -2.02102800 | -0.47161600 |
| C | 2.36118300 | 0.15729200 | -0.40481200 |
| C | 2.35079500 | -1.13385400 | -0.96237600 |
| C | 3.59074200 | 0.67717700 | 0.03934300 |
| C | 3.52570800 | -1.87306300 | -1.07804400 |
| H | 1.40819200 | -1.54179000 | -1.31185800 |
| C | 4.76572400 | -0.06429400 | -0.07391700 |
| H | 3.62272400 | 1.66180800 | 0.49785000 |
| C | 4.73997400 | -1.34286300 | -0.63444400 |
| H | 3.49508700 | -2.86545700 | -1.52083400 |
| H | 5.70227400 | 0.35518500 | 0.28453200 |
| H | 5.65580600 | -1.92112400 | -0.72248700 |
| C | 0.47167700 | -1.86486300 | 1.81072100 |
| H | 1.55438300 | -1.82496000 | 1.65880100 |
| H | 0.29553400 | -2.35457000 | 2.78391500 |
| H | 0.03626900 | -2.50778500 | 1.03951400 |
| C | 0.47262700 | 0.56621000 | 2.65334100 |
| H | 0.38061200 | 0.30994900 | 3.72200700 |
| H | 1.54294800 | 0.67673900 | 2.44302400 |
| H | -0.01264900 | 1.53710900 | 2.50664100 |
| H | -0.07748400 | 4.12064200 | -0.70980800 |

**R'=CF3, R=iPr**

Zero-point correction= 0.190042 (Hartree/Particle)
Thermal correction to Energy= 0.206264
Thermal correction to Enthalpy= 0.207208
Thermal correction to Gibbs Free Energy= 0.145177
Sum of electronic and zero-point Energies= -1040.626580
Sum of electronic and thermal Energies= -1040.610358
Sum of electronic and thermal Enthalpies= -1040.609414
Sum of electronic and thermal Free Energies= -1040.671445
Single-point electronic energy (M06) = -1040.6151

| | | | |
|---|---|---|---|
| C | -0.07882900 | -1.80418200 | 0.80090900 |
| H | -1.15934000 | -1.89533600 | 0.76182000 |
| C | -1.24566900 | 0.66184700 | 0.00144700 |
| C | 1.05581800 | 0.78040000 | -0.00228000 |
| C | -1.35389200 | 1.89224500 | 0.62974600 |
| C | 1.03420000 | 2.01168300 | 0.63892800 |
| C | -0.19109200 | 2.57472800 | 1.00562700 |
| H | -2.33444200 | 2.33032500 | 0.78414400 |
| H | 1.96345800 | 2.54651800 | 0.80152300 |
| N | -0.06028100 | 0.02250800 | -0.24260700 |
| C | 0.64287300 | -2.77570100 | -0.08150100 |
| H | 1.72096800 | -2.60189900 | -0.09624500 |
| H | 0.47884000 | -3.80202800 | 0.28557200 |
| H | 0.26149000 | -2.72612800 | -1.10575800 |
| C | 0.45807200 | -1.48213000 | 2.16208300 |
| H | 0.40128600 | -2.37256800 | 2.80982300 |
| H | 1.50766000 | -1.17662300 | 2.12713700 |
| H | -0.12587100 | -0.69291800 | 2.64866000 |
| H | -0.24041800 | 3.53442900 | 1.50795900 |
| C | 2.36904800 | 0.23814600 | -0.51604800 |
| C | -2.50534200 | -0.04435300 | -0.44527600 |
| F | 3.24976800 | 1.23943600 | -0.74165800 |
| F | 2.97967500 | -0.60430100 | 0.36606800 |
| F | 2.21930600 | -0.44540300 | -1.66282800 |
| F | -2.27531800 | -0.93482100 | -1.42327100 |
| F | -3.42406600 | 0.84100700 | -0.89256500 |
| F | -3.10078800 | -0.72007500 | 0.57778800 |

**R'=Cl, R=iPr**

Zero-point correction= 0.160874 (Hartree/Particle)
Thermal correction to Energy= 0.172553
Thermal correction to Enthalpy= 0.173497
Thermal correction to Gibbs Free Energy= 0.121748
Sum of electronic and zero-point Energies= -1285.776172
Sum of electronic and thermal Energies= -1285.764493
Sum of electronic and thermal Enthalpies= -1285.763549
Sum of electronic and thermal Free Energies= -1285.815298
Single-point electronic energy (M06) = -1285.7453

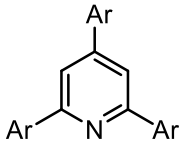
| | | | |
|---|---|---|---|
| C | 0.41507700 | -1.72321200 | 0.67741900 |
| H | -0.61426600 | -2.03795000 | 0.83558900 |
| C | -1.39083400 | 0.26511200 | -0.14398700 |
| C | 0.77711200 | 0.96009900 | -0.25064500 |
| C | -1.81074100 | 1.45106000 | 0.42806700 |
| C | 0.47720900 | 2.18569500 | 0.31692900 |
| C | -0.84598000 | 2.43021700 | 0.70596300 |
| H | -2.86534500 | 1.62029300 | 0.61378000 |
| H | 1.24882900 | 2.94119800 | 0.41327300 |
| N | -0.09769400 | -0.06831000 | -0.39994400 |
| C | 1.17560700 | -2.59608600 | -0.27598600 |
| H | 2.17337800 | -2.19969600 | -0.48569100 |
| H | 1.30050400 | -3.60434000 | 0.15130100 |
| H | 0.63842000 | -2.70231800 | -1.22350300 |
| C | 1.09922400 | -1.21743200 | 1.91278000 |
| H | 1.29909100 | -2.05304800 | 2.60312100 |
| H | 2.06397700 | -0.75103300 | 1.68620500 |
| H | 0.47857700 | -0.49395000 | 2.45316500 |
| H | -1.12411600 | 3.36796100 | 1.17478800 |
| Cl | 2.40313400 | 0.68891700 | -0.88534900 |
| Cl | -2.59697100 | -0.93254400 | -0.62321900 |

**R'=tBu, R=iPr**

Zero-point correction= 0.406663 (Hartree/Particle)
Thermal correction to Energy= 0.426629
Thermal correction to Enthalpy= 0.427573
Thermal correction to Gibbs Free Energy= 0.360668
Sum of electronic and zero-point Energies= -680.832042
Sum of electronic and thermal Energies= -680.812076
Sum of electronic and thermal Enthalpies= -680.811132
Sum of electronic and thermal Free Energies= -680.878037
Single-point electronic energy (M06) = -680.88171

| | | | |
|---|---|---|---|
| C | 0.13486800 | 1.82369300 | 0.80410000 |
| H | 1.22101000 | 1.86818800 | 0.80069000 |
| C | 1.24254800 | -0.53679100 | 0.20014100 |
| C | -1.11932600 | -0.61814700 | 0.17196000 |
| C | 1.28521500 | -1.54221300 | 1.15520300 |
| C | -1.10953400 | -1.61286000 | 1.14436000 |
| C | 0.09704200 | -2.04402800 | 1.70407100 |
| H | 2.23737700 | -1.98185000 | 1.43853600 |
| H | -2.03606900 | -2.10295700 | 1.42769900 |
| N | 0.04295700 | 0.08092100 | -0.13625000 |
| C | -0.47714400 | 2.93241500 | -0.00992500 |
| H | -1.56898400 | 2.87192500 | -0.04686900 |
| H | -0.22846400 | 3.90587400 | 0.44317100 |
| H | -0.09617200 | 2.94167500 | -1.03559900 |
| C | -0.42029100 | 1.60612000 | 2.18656200 |
| H | -0.30191400 | 2.52098400 | 2.78929300 |
| H | -1.48894400 | 1.36779300 | 2.16906000 |
| H | 0.10195500 | 0.79648000 | 2.70413100 |
| H | 0.11535100 | -2.80944700 | 2.47408800 |
| C | -2.40422400 | -0.32574000 | -0.63617800 |
| C | 2.52570800 | -0.12987700 | -0.55966700 |
| C | 3.62636700 | 0.35996700 | 0.41066400 |
| H | 4.54277300 | 0.59831100 | -0.14331300 |
| H | 3.31920500 | 1.26327600 | 0.95018900 |
| H | 3.87848200 | -0.40165600 | 1.15620200 |
| C | 2.27376300 | 0.95161800 | -1.62799700 |
| H | 2.01103200 | 1.91910100 | -1.19259300 |
| H | 3.18654900 | 1.09537400 | -2.21837800 |
| H | 1.46582200 | 0.66145300 | -2.30492800 |
| C | 3.04965900 | -1.38931700 | -1.30006200 |
| H | 3.95951200 | -1.14733200 | -1.86402000 |
| H | 3.29122300 | -2.20088400 | -0.60627800 |
| H | 2.30169500 | -1.76560000 | -2.00703200 |
| C | -2.08988400 | 0.42824200 | -1.94323600 |
| H | -3.01614800 | 0.57694200 | -2.51195400 |
| H | -1.63957100 | 1.40442800 | -1.76592800 |
| H | -1.39641800 | -0.14496900 | -2.56763700 |
| C | -3.43946100 | 0.46958400 | 0.19453600 |
| H | -4.36986800 | 0.59401200 | -0.37385000 |
| H | -3.68455000 | -0.05411400 | 1.12597300 |
| H | -3.07747200 | 1.46776400 | 0.45802100 |
| C | -3.06200800 | -1.67070900 | -1.04186400 |
| H | -3.42546900 | -2.23784600 | -0.17900100 |
| H | -3.92482100 | -1.47949000 | -1.69159600 |
| H | -2.35760000 | -2.30562300 | -1.59033700 |

## Pyridines




**Ar=Ph**

Zero-point correction= 0.332101 (Hartree/Particle)
Thermal correction to Energy= 0.350321
Thermal correction to Enthalpy= 0.351265
Thermal correction to Gibbs Free Energy= 0.283764
Sum of electronic and zero-point Energies= -941.131314
Sum of electronic and thermal Energies= -941.113094
Sum of electronic and thermal Enthalpies= -941.112150
Sum of electronic and thermal Free Energies= -941.179651
Single-point electronic energy (M06) = -940.96754439

| | | | |
|---|---|---|---|
| C | -0.76765100 | -1.19627000 | -0.01396800 |
| C | 0.63393200 | -1.15960600 | 0.00686500 |
| C | 0.63393200 | 1.15960500 | -0.00681100 |
| C | -0.76765000 | 1.19627000 | 0.01400600 |
| C | -1.49410700 | 0.00000000 | 0.00001700 |
| H | -1.29173400 | -2.14507500 | -0.02984500 |
| H | -1.29173100 | 2.14507700 | 0.02987100 |
| C | -2.97945200 | 0.00000100 | 0.00000700 |
| C | -3.69859900 | 0.93080800 | 0.76758900 |
| C | -3.69858500 | -0.93080900 | -0.76758900 |
| C | -5.09264500 | 0.92933400 | 0.76926300 |
| H | -3.16035500 | 1.64241600 | 1.38747400 |
| C | -5.09263000 | -0.92934000 | -0.76928500 |
| H | -3.16032800 | -1.64241500 | -1.38746600 |
| C | -5.79524500 | -0.00000400 | -0.00001600 |
| H | -5.63042400 | 1.65130000 | 1.37801300 |
| H | -5.63039800 | -1.65130700 | -1.37804200 |
| H | -6.88182600 | -0.00000700 | -0.00002400 |
| C | 1.44906100 | 2.40537400 | -0.01882800 |
| C | 0.93644300 | 3.62159700 | -0.49816600 |
| C | 2.77086900 | 2.37659600 | 0.45514100 |
| C | 1.71713500 | 4.77686300 | -0.49215100 |
| H | -0.06936600 | 3.66522200 | -0.90575300 |
| C | 3.54859500 | 3.53195200 | 0.46500500 |
| H | 3.17089900 | 1.43519900 | 0.81547500 |
| C | 3.02507400 | 4.73813800 | -0.00658200 |
| H | 1.30443500 | 5.70638300 | -0.87549200 |
| H | 4.56678700 | 3.49156600 | 0.84335800 |
| H | 3.63296000 | 5.63900500 | -0.00060700 |
| C | 1.44906400 | -2.40537400 | 0.01885400 |
| C | 2.77087100 | -2.37658000 | -0.45511900 |
| C | 0.93644700 | -3.62161400 | 0.49814700 |
| C | 3.54860200 | -3.53193100 | -0.46501300 |
| H | 3.17089600 | -1.43517000 | -0.81542600 |
| C | 1.71714300 | -4.77687700 | 0.49210000 |
| H | -0.06936400 | -3.66525800 | 0.90572700 |
| C | 3.02508400 | -4.73813200 | 0.00653800 |
| H | 4.56679400 | -3.49153300 | -0.84336400 |
| H | 1.30444500 | -5.70641000 | 0.87541100 |
| H | 3.63297400 | -5.63899600 | 0.00053800 |
| N | 1.31160300 | -0.00000100 | 0.00002000 |

**Ar=4-Me-Ph**

Zero-point correction= 0.414574 (Hartree/Particle)
Thermal correction to Energy= 0.438549
Thermal correction to Enthalpy= 0.439493
Thermal correction to Gibbs Free Energy= 0.356785
Sum of electronic and zero-point Energies= -1059.003663
Sum of electronic and thermal Energies= -1058.979688
Sum of electronic and thermal Enthalpies= -1058.978743
Sum of electronic and thermal Free Energies= -1059.061451
Single-point electronic energy (M06) = -1058.85333696

| | | | |
|---|---|---|---|
| C | -0.77901200 | -1.20299100 | -0.01099100 |
| C | 0.62247300 | -1.15703300 | 0.00861800 |
| C | 0.60661600 | 1.16258400 | -0.00789900 |
| C | -0.79531500 | 1.18935400 | 0.01370400 |
| C | -1.51408500 | -0.01179300 | 0.00171600 |
| H | -1.29652900 | -2.15545000 | -0.02442400 |
| H | -1.32580500 | 2.13464900 | 0.02809100 |
| C | -2.99847700 | -0.02120300 | 0.00199000 |
| C | -3.72869400 | 0.91072700 | 0.75717700 |
| C | -3.71759800 | -0.96378700 | -0.74912700 |
| C | -5.12103200 | 0.89687400 | 0.75984100 |
| H | -3.20003100 | 1.63342600 | 1.37265500 |
| C | -5.11077500 | -0.96968200 | -0.74667100 |
| H | -3.18117500 | -1.68482600 | -1.35978300 |
| C | -5.84001800 | -0.03971800 | 0.00494700 |
| H | -5.65965200 | 1.62190700 | 1.36624600 |
| H | -5.64142800 | -1.70739600 | -1.34455000 |
| C | 1.41195700 | 2.41331300 | -0.02204600 |

| | | | |
|---|---|---|---|
| C | 0.89186700 | 3.63063500 | -0.48755900 |
| C | 2.74079600 | 2.39688800 | 0.43155500 |
| C | 1.66749500 | 4.78819000 | -0.48587500 |
| H | -0.11751000 | 3.67568700 | -0.88634200 |
| C | 3.50851000 | 3.55698900 | 0.43490400 |
| H | 3.15782000 | 1.45804300 | 0.77931400 |
| C | 2.98724100 | 4.77719500 | -0.01822000 |
| H | 1.24171400 | 5.71508300 | -0.86421300 |
| H | 4.53407900 | 3.51628000 | 0.79623000 |
| C | 1.44500400 | -2.39652100 | 0.02176000 |
| C | 2.77250900 | -2.36185600 | -0.43480000 |
| C | 0.94295500 | -3.62059400 | 0.48927800 |
| C | 3.55630200 | -3.51110900 | -0.43899900 |
| H | 3.17565400 | -1.41753700 | -0.78410100 |
| C | 1.73471100 | -4.76722500 | 0.48681900 |
| H | -0.06485400 | -3.67939200 | 0.89024500 |
| C | 3.05312400 | -4.73812200 | 0.01627800 |
| H | 4.58041000 | -3.45640600 | -0.80262400 |
| H | 1.32278000 | -5.69967500 | 0.86682000 |
| N | 1.29248300 | 0.00740600 | -0.00015000 |
| C | 3.89935000 | -5.98875000 | -0.01781400 |
| H | 3.56657000 | -6.71905500 | 0.72736100 |
| H | 3.84684000 | -6.47845600 | -0.99975900 |
| H | 4.95441700 | -5.76493200 | 0.17449400 |
| C | 3.81569300 | 6.03967500 | 0.01520200 |
| H | 3.47479200 | 6.76348100 | -0.73266700 |
| H | 3.75338500 | 6.53100400 | 0.99577200 |
| H | 4.87433600 | 5.83031000 | -0.17356500 |
| C | -7.35031800 | -0.02921800 | -0.01551800 |
| H | -7.76298100 | 0.25674900 | 0.95815700 |
| H | -7.73301600 | 0.68963100 | -0.75254200 |
| H | -7.75486700 | -1.01189100 | -0.27939400 |

**Ar=4-MeO-Ph**

Zero-point correction= 0.430231 (Hartree/Particle)
Thermal correction to Energy= 0.456366
Thermal correction to Enthalpy= 0.457310
Thermal correction to Gibbs Free Energy= 0.371414
Sum of electronic and zero-point Energies= -1284.602968
Sum of electronic and thermal Energies= -1284.576833
Sum of electronic and thermal Enthalpies= -1284.575889
Sum of electronic and thermal Free Energies= -1284.661785
Single-point electronic energy (M06) = -1284.45413195

| | | | |
|---|---|---|---|
| C | 0.98612300 | 1.07011500 | 0.05273300 |
| C | -0.41291000 | 1.16825500 | 0.04699600 |
| C | -0.63395300 | -1.14154400 | -0.01429900 |
| C | 0.75766000 | -1.31161800 | 0.02715600 |
| C | 1.59608500 | -0.19038400 | 0.05158800 |
| H | 1.59900400 | 1.96401400 | 0.07077900 |
| H | 1.18887000 | -2.30607500 | 0.02890300 |
| C | 3.07223800 | -0.33307300 | 0.07514400 |
| C | 3.69292100 | -1.37231300 | 0.79452200 |
| C | 3.90028000 | 0.55935200 | -0.61821000 |
| C | 5.07289900 | -1.50900200 | 0.82034900 |
| H | 3.08304300 | -2.06734500 | 1.36470300 |
| C | 5.29025100 | 0.43332900 | -0.60638800 |
| H | 3.45401000 | 1.35717700 | -1.20534500 |
| C | 5.88543000 | -0.60624600 | 0.11787400 |
| H | 5.54923000 | -2.30350300 | 1.38627000 |
| H | 5.89120100 | 1.13937300 | -1.16807900 |
| C | -1.56307200 | -2.30054400 | -0.06275800 |
| C | -1.15824700 | -3.57246200 | -0.50894800 |
| C | -2.89632600 | -2.14735100 | 0.34047100 |
| C | -2.04169400 | -4.64188200 | -0.53821300 |
| H | -0.14427800 | -3.72834900 | -0.86513000 |
| C | -3.79526900 | -3.21277800 | 0.32090500 |
| H | -3.22381100 | -1.17020000 | 0.67814300 |
| C | -3.36919000 | -4.47226800 | -0.11863500 |
| H | -1.72997400 | -5.61976100 | -0.89184500 |
| H | -4.81552100 | -3.05199600 | 0.65073400 |
| C | -1.10547400 | 2.48311100 | 0.07063300 |
| C | -2.42994700 | 2.58649000 | -0.37518800 |
| C | -0.48038500 | 3.65503500 | 0.53598600 |
| C | -3.11002800 | 3.80352700 | -0.37736400 |
| H | -2.92654800 | 1.68936800 | -0.72831200 |
| C | -1.14470100 | 4.87303300 | 0.54394800 |
| H | 0.53273500 | 3.61506400 | 0.92492200 |
| C | -2.46653400 | 4.95899200 | 0.08295900 |
| H | -4.13129600 | 3.83965100 | -0.73967000 |
| H | -0.66411000 | 5.77373200 | 0.91309000 |
| N | -1.19784100 | 0.07820300 | 0.00459000 |
| O | -3.03151100 | 6.20052200 | 0.12809000 |
| O | 7.22861300 | -0.82576200 | 0.20345500 |
| O | -4.15797300 | -5.58427200 | -0.18021500 |
| C | 8.09974500 | 0.06450200 | -0.47654300 |
| H | 9.11101700 | -0.28965100 | -0.26872500 |
| H | 7.92624600 | 0.04987700 | -1.56066200 |
| H | 7.99259800 | 1.09332700 | -0.10821300 |
| C | -4.37318800 | 6.34340200 | -0.30993700 |
| H | -4.61893300 | 7.39934500 | -0.18235500 |
| H | -4.48439700 | 6.07074600 | -1.36783100 |
| H | -5.06147400 | 5.73557300 | 0.29216900 |
| C | -5.51375600 | -5.46831300 | 0.22060200 |
| H | -5.95063100 | -6.46004800 | 0.08914800 |
| H | -5.59989000 | -5.17126400 | 1.27424200 |
| H | -6.05899000 | -4.74659100 | -0.40198800 |

**Ar=4-CF3-Ph**

Zero-point correction= 0.346222 (Hartree/Particle)
Thermal correction to Energy= 0.375484
Thermal correction to Enthalpy= 0.376428
Thermal correction to Gibbs Free Energy= 0.279721
Sum of electronic and zero-point Energies= -1952.229041
Sum of electronic and thermal Energies= -1952.199778
Sum of electronic and thermal Enthalpies= -1952.198834
Sum of electronic and thermal Free Energies= -1952.295541
Single-point electronic energy (M06) = -1952.07201957

| | | | |
|---|---|---|---|
| C | -0.79429300 | -1.22623700 | 0.00639200 |
| C | 0.60566800 | -1.15155000 | 0.02177700 |
| C | 0.54498500 | 1.16528200 | -0.01135000 |
| C | -0.85680700 | 1.16679000 | 0.01400200 |
| C | -1.55041200 | -0.04867000 | 0.01268000 |
| H | -1.29367900 | -2.18831000 | 0.00060300 |
| H | -1.40559600 | 2.10155200 | 0.02352100 |
| C | -3.03501700 | -0.08665200 | 0.01756800 |
| C | -3.77443600 | 0.82481200 | 0.78873700 |
| C | -3.73237400 | -1.03665000 | -0.74610000 |
| C | -5.16573200 | 0.78967600 | 0.79693000 |
| H | -3.25535700 | 1.54850900 | 1.41009300 |
| C | -5.12374200 | -1.07294800 | -0.74405400 |
| H | -3.18141400 | -1.73786900 | -1.36572300 |
| C | -5.84453400 | -0.15930500 | 0.02867300 |
| H | -5.72463000 | 1.48868400 | 1.41021400 |
| H | -5.65007900 | -1.80989800 | -1.34155400 |
| C | 1.32837400 | 2.43089500 | -0.03616900 |
| C | 0.78286600 | 3.62994100 | -0.52118200 |
| C | 2.65410900 | 2.43756500 | 0.42726800 |
| C | 1.53118800 | 4.80383800 | -0.52857100 |
| H | -0.22415300 | 3.64852100 | -0.92609600 |
| C | 3.40389500 | 3.60846300 | 0.42451600 |
| H | 3.08348900 | 1.51009300 | 0.78857900 |
| C | 2.84339500 | 4.79765000 | -0.05120000 |
| H | 1.10195800 | 5.72046300 | -0.91902200 |
| H | 4.42687100 | 3.60049500 | 0.78662500 |
| C | 1.45492100 | -2.37403000 | 0.04082800 |
| C | 2.77547500 | -2.31019700 | -0.43316300 |
| C | 0.97815100 | -3.59994700 | 0.53085800 |
| C | 3.58675800 | -3.43920400 | -0.43528800 |
| H | 3.15187200 | -1.36146200 | -0.79829800 |
| C | 1.78835000 | -4.73222900 | 0.53343400 |
| H | -0.02334600 | -3.67189300 | 0.94347500 |
| C | 3.09448400 | -4.65619900 | 0.04586400 |

| | | | |
|---|---|---|---|
| H | 4.60510900 | -3.37688000 | -0.80518500 |
| H | 1.41192600 | -5.66997800 | 0.92811800 |
| N | 1.25251800 | 0.02458900 | 0.00281400 |
| C | 3.95470200 | -5.88912300 | -0.01166400 |
| C | -7.34926000 | -0.15885600 | -0.01196800 |
| C | 3.63463400 | 6.07607400 | 0.00188400 |
| F | 3.60434300 | -6.79462200 | 0.92855500 |
| F | 3.85602800 | -6.51028000 | -1.21094100 |
| F | 5.26203800 | -5.59820700 | 0.17023000 |
| F | -7.84573000 | -1.39336800 | -0.24631900 |
| F | -7.88244700 | 0.28242600 | 1.14850400 |
| F | -7.81955600 | 0.64704800 | -0.99244700 |
| F | 4.95677100 | 5.85696600 | -0.17291200 |
| F | 3.49614000 | 6.69849700 | 1.19662300 |
| F | 3.23878200 | 6.95495200 | -0.94565400 |

**Ar=4-F-Ph**

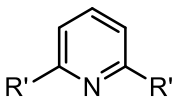
Zero-point correction= 0.307295 (Hartree/Particle)
Thermal correction to Energy= 0.328101
Thermal correction to Enthalpy= 0.329045
Thermal correction to Gibbs Free Energy= 0.255143
Sum of electronic and zero-point Energies= -1238.856473
Sum of electronic and thermal Energies= -1238.835667
Sum of electronic and thermal Enthalpies= -1238.834723
Sum of electronic and thermal Free Energies= -1238.908625
Single-point electronic energy (M06) = -1238.69155330

| | | | |
|---|---|---|---|
| C | 0.78913700 | -1.19650300 | 0.01379200 |
| C | -0.61239600 | -1.15975900 | -0.00708300 |
| C | -0.61254500 | 1.15970300 | 0.00685300 |
| C | 0.78899200 | 1.19665900 | -0.01378500 |
| C | 1.51525000 | 0.00012600 | 0.00002700 |
| H | 1.31381000 | -2.14504300 | 0.02919000 |
| H | 1.31350500 | 2.14528700 | -0.02901300 |
| C | 2.99985000 | 0.00014900 | 0.00008200 |
| C | 3.72071900 | 0.93399400 | -0.76325400 |
| C | 3.72080000 | -0.93364300 | 0.76335600 |
| C | 5.11375400 | 0.93979900 | -0.77036200 |
| H | 3.18554100 | 1.64916100 | -1.38090700 |
| C | 5.11382000 | -0.93923600 | 0.77033300 |
| H | 3.18581300 | -1.64893300 | 1.38103900 |
| C | 5.78941800 | 0.00031400 | -0.00002200 |
| H | 5.67665700 | 1.65049600 | -1.36639400 |
| H | 5.67699200 | -1.64980900 | 1.36626900 |
| C | -1.42897700 | 2.40316300 | 0.01873200 |
| C | -0.91802900 | 3.62402400 | 0.48898200 |
| C | -2.75504200 | 2.36953400 | -0.44530400 |
| C | -1.69521800 | 4.78057800 | 0.48677500 |
| H | 0.08977500 | 3.67594000 | 0.88932500 |
| C | -3.54301400 | 3.51646900 | -0.45777400 |
| H | -3.15636400 | 1.42657300 | -0.79903100 |
| C | -2.99786800 | 4.70815900 | 0.00803400 |
| H | -1.31070300 | 5.72501600 | 0.85749800 |
| H | -4.56485900 | 3.50107600 | -0.82279400 |
| C | -1.42867200 | -2.40332000 | -0.01883500 |
| C | -2.75480700 | -2.36976500 | 0.44501200 |
| C | -0.91750900 | -3.62420900 | -0.48877300 |
| C | -3.54264800 | -3.51678800 | 0.45757100 |
| H | -3.15629200 | -1.42678400 | 0.79849900 |
| C | -1.69456200 | -4.78085400 | -0.48646600 |
| H | 0.09036100 | -3.67608200 | -0.88895700 |
| C | -2.99729000 | -4.70850100 | -0.00792900 |
| H | -4.56455400 | -3.50144800 | 0.82242400 |
| H | -1.30988100 | -5.72531300 | -0.85696500 |
| N | -1.29002100 | -0.00006900 | -0.00013500 |
| F | -3.75503600 | -5.82471300 | -0.00007600 |
| F | -3.75573000 | 5.82429100 | 0.00024600 |
| F | 7.13758400 | 0.00039800 | -0.00006100 |

**Ar=3,5-diF-Ph**

Zero-point correction= 0.282248 (Hartree/Particle)
Thermal correction to Energy= 0.305701
Thermal correction to Enthalpy= 0.306645
Thermal correction to Gibbs Free Energy= 0.226401
Sum of electronic and zero-point Energies= -1536.577612
Sum of electronic and thermal Energies= -1536.554160
Sum of electronic and thermal Enthalpies= -1536.553216
Sum of electronic and thermal Free Energies= -1536.633459
Single-point electronic energy (M06) = -1536.40995294

| | | | |
|---|---|---|---|
| C | 0.79092700 | -1.19717400 | 0.00888100 |
| C | -0.61009400 | -1.15847100 | -0.01160800 |
| C | -0.60996400 | 1.15848100 | 0.01159500 |
| C | 0.79106500 | 1.19705200 | -0.00881700 |
| C | 1.51502500 | -0.00009900 | 0.00003800 |
| H | 1.31616900 | -2.14509300 | 0.02037400 |
| H | 1.31637800 | 2.14493200 | -0.02025500 |
| C | 3.00079900 | -0.00022000 | 0.00005000 |
| C | 3.70935600 | 0.93725400 | -0.76753400 |
| C | 3.70930700 | -0.93769100 | 0.76755400 |
| C | 5.09823700 | 0.91435500 | -0.75193800 |
| H | 3.19903600 | 1.65841900 | -1.39579300 |
| C | 5.09823600 | -0.91480400 | 0.75178600 |
| H | 3.19911800 | -1.65889200 | 1.39588700 |
| C | 5.82646400 | -0.00024700 | -0.00010800 |
| C | -1.42785900 | 2.40319200 | 0.02837400 |
| C | -0.89565600 | 3.62226900 | 0.47720000 |
| C | -2.75942700 | 2.35402800 | -0.41085800 |
| C | -1.69817000 | 4.75554400 | 0.46759600 |
| H | 0.11395100 | 3.70568500 | 0.86168600 |
| C | -3.51681700 | 3.51623400 | -0.40420900 |
| H | -3.18998200 | 1.42134500 | -0.75241700 |
| C | -3.01629400 | 4.73977200 | 0.02867000 |
| C | -1.42814100 | -2.40308300 | -0.02834800 |
| C | -2.75977500 | -2.35368500 | 0.41066400 |
| C | -0.89604400 | -3.62228800 | -0.47695500 |
| C | -3.51732700 | -3.51578500 | 0.40403100 |
| H | -3.19025300 | -1.42090000 | 0.75204100 |
| C | -1.69871500 | -4.75545000 | -0.46733400 |
| H | 0.11360500 | -3.70589800 | -0.86128500 |
| C | -3.01690400 | -4.73944600 | -0.02861500 |
| N | -1.28676700 | 0.00004600 | -0.00001300 |
| H | 6.90973200 | -0.00040500 | -0.00003100 |
| H | -3.62644100 | -5.63497400 | -0.02847300 |
| H | -3.62570600 | 5.63538500 | 0.02854100 |
| F | -4.79145500 | 3.46455100 | -0.83710000 |
| F | -1.18006800 | 5.91873900 | 0.90940100 |
| F | -4.79202500 | -3.46387200 | 0.83671800 |
| F | -1.18070900 | -5.91876700 | -0.90893200 |
| F | 5.76893900 | 1.80913200 | -1.50093000 |
| F | 5.76891700 | -1.80960100 | 1.50074500 |




**R'=H**

Zero-point correction= 0.089031 (Hartree/Particle)
Thermal correction to Energy= 0.093300
Thermal correction to Enthalpy= 0.094244
Thermal correction to Gibbs Free Energy= 0.061630
Sum of electronic and zero-point Energies= -248.195942
Sum of electronic and thermal Energies= -248.191673
Sum of electronic and thermal Enthalpies= -248.190729
Sum of electronic and thermal Free Energies= -248.223343
Single-point electronic energy (M06) =

-

248.15741

| | | | |
|---|---|---|---|
| C | -1.14254700 | -0.72168300 | 0.00009600 |
| C | 1.14209000 | -0.72239800 | 0.00010200 |
| C | -1.19846000 | 0.67342700 | 0.00003400 |
| C | 1.19887900 | 0.67272800 | 0.00002600 |

| | | | |
|---|---|---|---|
| C | 0.00043400 | 1.38561100 | -0.00019300 |
| H | -2.15737300 | 1.18342400 | 0.00027100 |
| H | 2.15812200 | 1.18208800 | 0.00023900 |
| N | -0.00043900 | -1.42100500 | -0.00024600 |
| H | -2.06044400 | -1.30796700 | 0.00035600 |
| H | 2.05966200 | -1.30920600 | 0.00039700 |
| H | 0.00073100 | 2.47257800 | 0.00006400 |

**R'=Me**

Zero-point correction= 0.143931 (Hartree/Particle)
Thermal correction to Energy= 0.151865
Thermal correction to Enthalpy= 0.152809
Thermal correction to Gibbs Free Energy= 0.110133
Sum of electronic and zero-point Energies= -326.782652
Sum of electronic and thermal Energies= -326.774718
Sum of electronic and thermal Enthalpies= -326.773774
Sum of electronic and thermal Free Energies= -326.816450
Single-point electronic energy (M06) =

-

326.75408

| | | | |
|---|---|---|---|
| C | -1.15719800 | -0.26557900 | -0.00000100 |
| C | 1.15717700 | -0.26560400 | -0.00006600 |
| C | -1.19986800 | 1.13439200 | 0.00004700 |
| C | 1.19987600 | 1.13439500 | -0.00004700 |
| C | 0.00001500 | 1.84127700 | 0.00001400 |
| H | -2.15416700 | 1.65311400 | 0.00009500 |
| H | 2.15419600 | 1.65307600 | -0.00008400 |
| N | -0.00000400 | -0.94599700 | -0.00005700 |
| H | 0.00000000 | 2.92846100 | 0.00003100 |
| C | -2.41786000 | -1.09593900 | 0.00000200 |
| H | -2.44588600 | -1.74813000 | -0.88029500 |
| H | -2.44597700 | -1.74800400 | 0.88039100 |
| H | -3.31623100 | -0.47119300 | -0.00008300 |
| C | 2.41785700 | -1.09594500 | 0.00004600 |
| H | 2.44660500 | -1.74696800 | 0.88119900 |
| H | 2.44527800 | -1.74918100 | -0.87948500 |
| H | 3.31621200 | -0.47118200 | -0.00134600 |

**R'=Ph**

Zero-point correction= 0.251122 (Hartree/Particle)
Thermal correction to Energy= 0.264555
Thermal correction to Enthalpy= 0.265499
Thermal correction to Gibbs Free Energy= 0.209552
Sum of electronic and zero-point Energies= -710.154467
Sum of electronic and thermal Energies= -710.141034
Sum of electronic and thermal Enthalpies= -710.140090
Sum of electronic and thermal Free Energies= -710.196037
Single-point electronic energy (M06) =

-

710.02588

| | | | |
|---|---|---|---|
| C | 1.20117700 | 2.25246500 | 0.03539700 |
| C | 1.16336700 | 0.84818700 | 0.01452400 |
| C | -1.16336700 | 0.84818700 | -0.01452500 |
| C | -1.20117700 | 2.25246500 | -0.03539700 |
| C | 0.00000000 | 2.95329700 | 0.00000000 |
| H | 2.14543200 | 2.78228400 | 0.09521800 |
| H | -2.14543300 | 2.78228400 | -0.09521800 |
| C | -2.40478500 | 0.02760600 | -0.03195600 |
| C | -3.63432900 | 0.53832100 | 0.41440400 |
| C | -2.36016700 | -1.29555200 | -0.50091700 |
| C | -4.78686200 | -0.24563200 | 0.38191200 |
| H | -3.69106400 | 1.54581200 | 0.81627700 |
| C | -3.51267600 | -2.07667000 | -0.53717500 |
| H | -1.40902300 | -1.69367500 | -0.83692100 |
| C | -4.73189300 | -1.55510800 | -0.09796600 |
| H | -5.72714700 | 0.16569300 | 0.73957500 |
| H | -3.46003000 | -3.09588200 | -0.91123200 |
| H | -5.63057700 | -2.16563700 | -0.12495700 |
| C | 2.40478600 | 0.02760600 | 0.03195500 |
| C | 2.36016600 | -1.29555300 | 0.50091500 |
| C | 3.63433000 | 0.53832100 | -0.41440300 |
| C | 3.51267500 | -2.07667100 | 0.53717400 |
| H | 1.40902200 | -1.69367500 | 0.83691800 |
| C | 4.78686300 | -0.24563200 | -0.38190900 |
| H | 3.69106500 | 1.54581300 | -0.81627400 |
| C | 4.73189300 | -1.55510900 | 0.09796800 |
| H | 3.46002900 | -3.09588300 | 0.91123000 |
| H | 5.72714800 | 0.16569300 | -0.73957100 |
| H | 5.63057600 | -2.16563800 | 0.12495900 |
| N | 0.00000000 | 0.17706200 | -0.00000100 |
| H | 0.00000000 | 4.04020800 | 0.00000000 |

**R'=CF3**

Zero-point correction= 0.098393 (Hartree/Particle)
Thermal correction to Energy= 0.109798
Thermal correction to Enthalpy= 0.110742
Thermal correction to Gibbs Free Energy= 0.057051
Sum of electronic and zero-point Energies= -922.255939
Sum of electronic and thermal Energies= -922.244534
Sum of electronic and thermal Enthalpies= -922.243590
Sum of electronic and thermal Free Energies= -922.297281
Single-point electronic energy (M06) =

-

922.22041

| | | | |
|---|---|---|---|
| C | -1.13937200 | 0.36533700 | 0.00007300 |
| C | 1.13936500 | 0.36530000 | -0.00030200 |
| C | -1.20120400 | 1.75977500 | 0.00017400 |
| C | 1.20125300 | 1.75977500 | -0.00021300 |
| C | 0.00004100 | 2.46599400 | 0.00000500 |
| H | -2.15779000 | 2.26795200 | 0.00035500 |
| H | 2.15787100 | 2.26789200 | -0.00034600 |
| N | 0.00000500 | -0.32672900 | -0.00015100 |
| H | 0.00002700 | 3.55185000 | 0.00007400 |
| C | -2.40050700 | -0.47964500 | 0.00005200 |
| C | 2.40049500 | -0.47968600 | 0.00000200 |
| F | -2.45739100 | -1.26948800 | -1.08668800 |
| F | -3.50741700 | 0.29855900 | 0.00042500 |
| F | -2.45712100 | -1.27026100 | 1.08611700 |
| F | 2.45620800 | -1.27190900 | -1.08498900 |
| F | 2.45827700 | -1.26787200 | 1.08784300 |
| F | 3.50738100 | 0.29856100 | -0.00245900 |

**R'=Cl**

Zero-point correction= 0.069558 (Hartree/Particle)
Thermal correction to Energy= 0.076079
Thermal correction to Enthalpy= 0.077024
Thermal correction to Gibbs Free Energy= 0.037619
Sum of electronic and zero-point Energies= -1167.409711
Sum of electronic and thermal Energies= -1167.403190
Sum of electronic and thermal Enthalpies= -1167.402246
Sum of electronic and thermal Free Energies= -1167.441651
Single-point electronic energy (M06) =

-

1167.3518

| | | | |
|---|---|---|---|
| C | -1.13015500 | 0.00428900 | 0.00059100 |
| C | 1.13012700 | 0.00425100 | 0.00049600 |
| C | -1.20613300 | 1.39778300 | 0.00025900 |
| C | 1.20612300 | 1.39778800 | 0.00018000 |
| C | 0.00001000 | 2.09656000 | -0.00061300 |
| H | -2.16447100 | 1.90262000 | 0.00034200 |
| H | 2.16450100 | 1.90254500 | 0.00020300 |
| N | -0.00001400 | -0.68516700 | -0.00037500 |
| H | -0.00001900 | 3.18282400 | -0.00048400 |
| Cl | -2.61901400 | -0.92929500 | -0.00010300 |
| Cl | 2.61902900 | -0.92928400 | -0.00006900 |

**R'=tBu**

Zero-point correction= 0.314735 (Hartree/Particle)

Thermal correction to Energy= 0.330041
Thermal correction to Enthalpy= 0.330986
Thermal correction to Gibbs Free Energy= 0.273329
Sum of electronic and zero-point Energies= -562.490393
Sum of electronic and thermal Energies= -562.475086
Sum of electronic and thermal Enthalpies= -562.474142
Sum of electronic and thermal Free Energies= -562.531799
Single-point electronic energy (M06) =

-

562.50686

| | | | |
|---|---|---|---|
| C | -1.16641800 | 0.42507300 | 0.00002300 |
| C | 1.16641800 | 0.42507500 | -0.00001600 |
| C | -1.20346700 | 1.82590500 | 0.00001900 |
| C | 1.20346100 | 1.82591400 | -0.00001100 |
| C | -0.00000300 | 2.52602900 | 0.00000100 |
| H | -2.14492500 | 2.36213000 | 0.00003500 |
| H | 2.14492200 | 2.36213300 | -0.00002100 |
| N | 0.00000300 | -0.23906600 | 0.00000700 |
| H | -0.00001200 | 3.61341500 | -0.00000900 |
| C | -2.42719400 | -0.45546900 | 0.00000400 |
| C | 2.42719600 | -0.45546700 | 0.00000300 |
| C | -3.72354700 | 0.37372600 | 0.00001100 |
| H | -4.59030300 | -0.29669900 | -0.00003700 |
| H | -3.80174000 | 1.01159700 | 0.88837100 |
| H | -3.80169600 | 1.01167600 | -0.88829500 |
| C | -2.40312500 | -1.35043900 | -1.25989100 |
| H | -1.48813500 | -1.94794400 | -1.28988300 |
| H | -3.26486800 | -2.02900000 | -1.26157300 |
| H | -2.44610700 | -0.74623400 | -2.17415100 |
| C | -2.40312900 | -1.35049600 | 1.25984600 |
| H | -2.44613900 | -0.74634700 | 2.17414600 |
| H | -3.26485300 | -2.02908400 | 1.26149600 |
| H | -1.48812800 | -1.94798700 | 1.28983000 |
| C | 2.40309700 | -1.35051200 | -1.25983800 |
| H | 3.26481800 | -2.02910100 | -1.26148400 |
| H | 1.48808800 | -1.94799000 | -1.28979600 |
| H | 2.44609900 | -0.74636000 | -2.17413400 |
| C | 3.72356300 | 0.37371500 | -0.00005500 |
| H | 3.80174300 | 1.01168900 | 0.88823200 |
| H | 4.59031200 | -0.29672000 | -0.00000400 |
| H | 3.80175200 | 1.01155700 | -0.88843500 |
| C | 2.40314300 | -1.35041500 | 1.25990100 |
| H | 3.26484200 | -2.02903600 | 1.26155700 |
| H | 2.44622000 | -0.74620300 | 2.17415600 |
| H | 1.48811900 | -1.94786500 | 1.28997000 |

**iPr radical**

Zero-point correction= 0.088607 (Hartree/Particle)
Thermal correction to Energy= 0.093743
Thermal correction to Enthalpy= 0.094687
Thermal correction to Gibbs Free Energy= 0.061414
Sum of electronic and zero-point Energies= -118.389546
Sum of electronic and thermal Energies= -118.384410
Sum of electronic and thermal Enthalpies= -118.383466
Sum of electronic and thermal Free Energies= -118.416739
Single-point electronic energy (M06, dioxane) = -118.40388
(M06, DMF) = -118.4047906

| | | | |
|---|---|---|---|
| C | 0.00000000 | 0.53171400 | -0.05308700 |
| H | 0.00000000 | 1.60552600 | 0.12080200 |
| C | -1.30116800 | -0.19768700 | 0.00372000 |
| H | -1.52795400 | -0.57058200 | 1.02006600 |
| H | -2.14157400 | 0.44011800 | -0.29321000 |
| H | -1.29744500 | -1.08132300 | -0.65031200 |
| C | 1.30116800 | -0.19768700 | 0.00372000 |
| H | 1.29744600 | -1.08132000 | -0.65031600 |
| H | 2.14157500 | 0.44011900 | -0.29320600 |
| H | 1.52795200 | -0.57058600 | 1.02006500 |

**Cy radical**

Zero-point correction= 0.156344 (Hartree/Particle)
Thermal correction to Energy= 0.162374
Thermal correction to Enthalpy= 0.163318
Thermal correction to Gibbs Free Energy= 0.126621
Sum of electronic and zero-point Energies= -235.057573
Sum of electronic and thermal Energies= -235.051542
Sum of electronic and thermal Enthalpies= -235.050598
Sum of electronic and thermal Free Energies= -235.087295
Single-point electronic energy (M06) = -235.08084

| | | | |
|---|---|---|---|
| C | -0.00001400 | 1.46430000 | -0.16685600 |
| C | 1.29089700 | 0.77842400 | 0.15640000 |
| C | -1.29091300 | 0.77840200 | 0.15639900 |
| H | -0.00002200 | 2.53025400 | -0.38200200 |
| C | 1.26829900 | -0.71304900 | -0.24239900 |
| H | 1.48483400 | 0.83687900 | 1.24649500 |
| H | 2.13564500 | 1.29023600 | -0.32199100 |
| C | -1.26828500 | -0.71307200 | -0.24239700 |
| H | -1.48485400 | 0.83685500 | 1.24649300 |
| H | -2.13566900 | 1.29019700 | -0.32199500 |
| C | 0.00001300 | -1.41137800 | 0.27081800 |
| H | 2.16541800 | -1.21644500 | 0.13990200 |
| H | 1.30183300 | -0.79145900 | -1.33804600 |
| H | -2.16539400 | -1.21648400 | 0.13990500 |
| H | -1.30182000 | -0.79148200 | -1.33804400 |
| H | 0.00002400 | -2.46586000 | -0.03408200 |
| H | 0.00001500 | -1.40445000 | 1.37157200 |

# Relative Contributions of Sterics and Electronics (Eq 3)

Parameters were normalized using average values of each range and standard deviation as:

$$p_{i\,norm} = \frac{(p_i - \bar{p})}{\sigma}$$

Bilinear regression analysis performed with normalized parameters in MS Excel returned the following:

Bilinear fit with normalzied parameters

| | σ | ν | | Prediction |
|---|---|---|---|---|
| H | -0.25556 | -1.65933 | 1.2 | 1.265348 |
| Me | -0.92394 | -0.29334 | -11.4 | -9.69852 |
| Ph | -0.29487 | -0.16199 | -5.1 | -8.92137 |
| $CF_3$ | 1.867538 | 0.731156 | -9 | -9.22395 |
| Cl | 0.648724 | -0.21453 | -8 | -6.07518 |
| tBu | -1.04189 | 1.598036 | -23.1 | -22.7463 |

SUMMARY OUTPUT

*Regression Statistics*

| | |
|---|---|
| Multiple R | 0.966491 |
| R Square | 0.934105 |
| Adjusted R | 0.890176 |
| Standard E | 2.66973 |
| Observatic | 6 |

ANOVA

| | *df* | *SS* | *MS* | *F* | *ignificance F* |
|---|---|---|---|---|---|
| Regressior | 2 | 303.111 | 151.5555 | 21.2636 | 0.016915 |
| Residual | 3 | 21.38238 | 7.12746 | | |
| Total | 5 | 324.4933 | | | |

| | *Coefficients* | *andard Erı* | *t Stat* | *P-value* | *Lower 95%* | *Upper 95%* | *ower 95.0%* | *pper 95.0%* |
|---|---|---|---|---|---|---|---|---|
| Intercept | -9.23333 | 1.089913 | -8.47163 | 0.003453 | -12.7019 | -5.76474 | -12.7019 | -5.76474 |
| X Variable | 2.641386 | 1.091316 | 2.420367 | 0.094138 | -0.83167 | 6.11444 | -0.83167 | 6.11444 |
| X Variable | -6.73386 | 1.091316 | -6.17041 | 0.008569 | -10.2069 | -3.26081 | -10.2069 | -3.26081 |

Coefficients for Hammett (2.64) and Charton (-6.73) parameters indicate that ~25% of variance in the thermodynamics of dissociation can be ascribed to the electronic factors, while rest of the energetics results from sterics.

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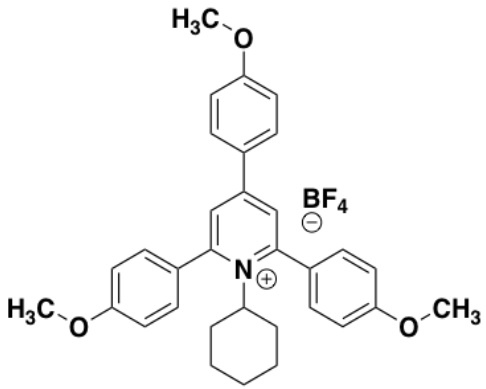
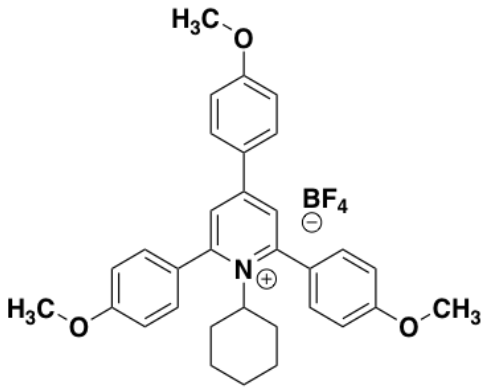


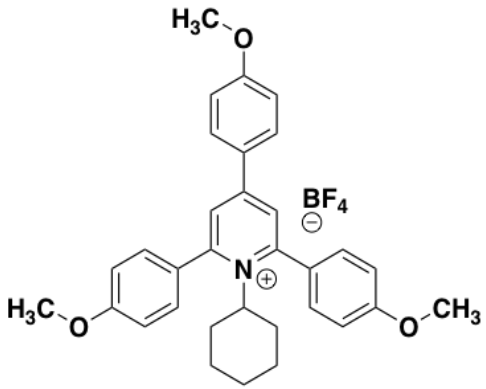

Compound **1a-Cy**

$^1$H NMR (600 MHz, $CDCl_3$)



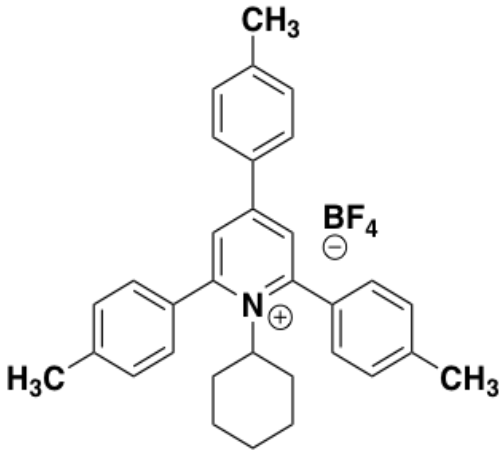

Compound **1a-Cy**

$^{13}C$ NMR (151 MHz, $CDCl_3$)



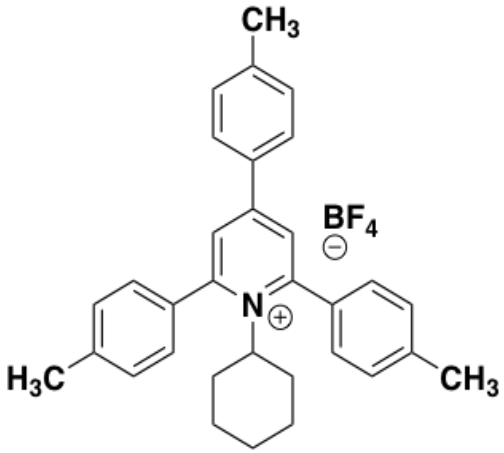

Compound **1a-Cy**

$^{19}F$ NMR (376 MHz, $CDCl_3$)



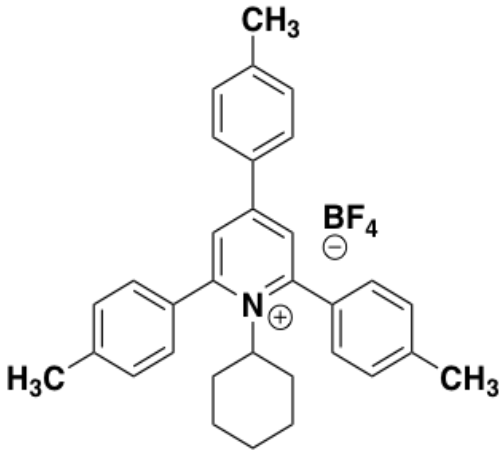

Compound **1b-Cy**

$^1$H NMR (600 MHz, $CDCl_3$)



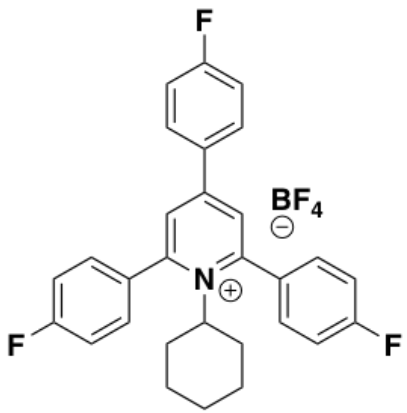

Compound **1b-Cy**

$^{13}C$ NMR (151 MHz, $CDCl_3$)



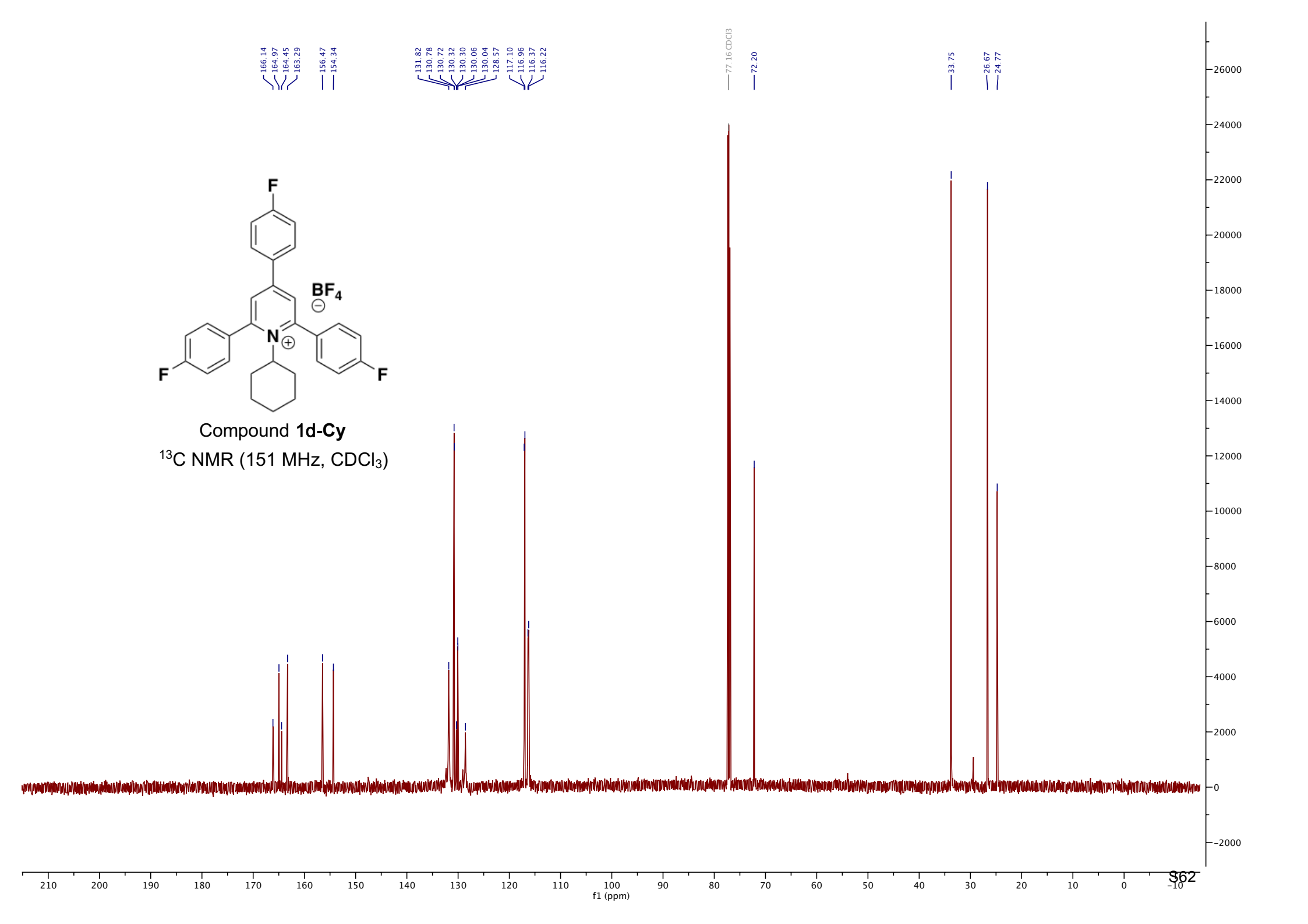

Compound **1b-Cy**

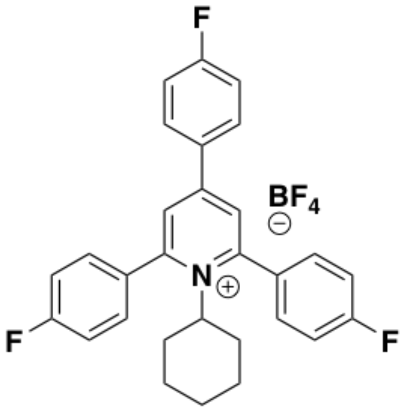
$^{19}F$ NMR (376 MHz, $CDCl_3$)




Compound **1d-Cy**

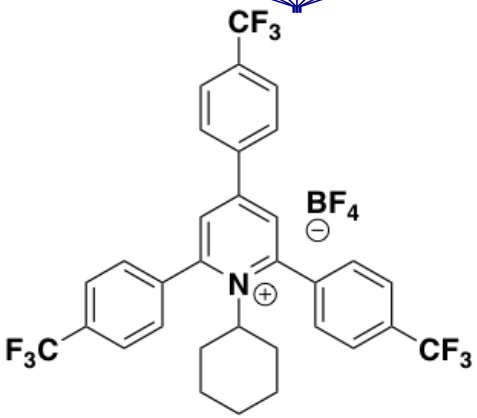
$^1$H NMR (600 MHz, $CDCl_3$)


166.14
164.97
164.45
163.29
156.47
154.34
131.82
130.78
130.72
130.32
130.30
130.06
130.04
128.57
117.10
116.96
116.37
116.22
77.16 CDCl3
72.20
33.75
26.67
24.77
F
BF4
N
F
F
Compound 1d-Cy
13C NMR (151 MHz, CDCl3)
f1 (ppm)



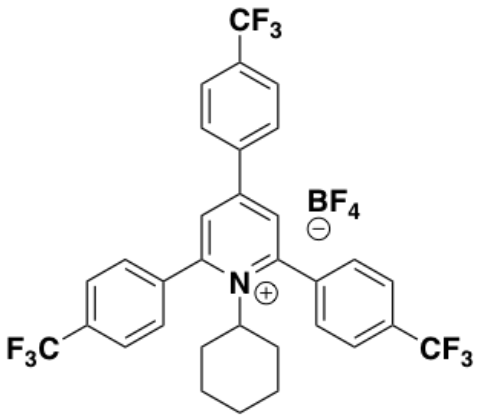

Compound **1d-Cy**

$^{19}F$ NMR (376 MHz, $CDCl_3$)



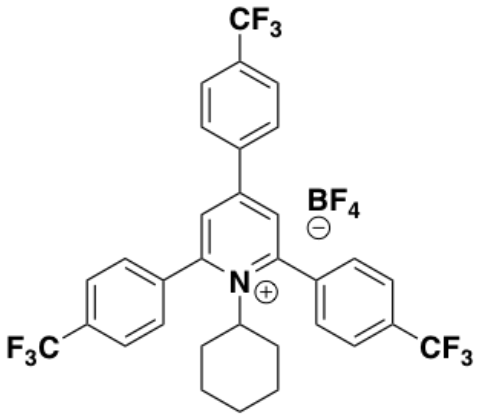

Compound **1e-Cy**

$^1$H NMR (600 MHz, $CDCl_3$)



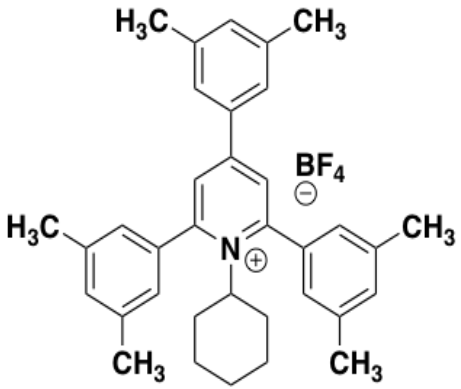

Compound **1e-Cy**

$^{13}C$ NMR (151 MHz, $CDCl_3$)



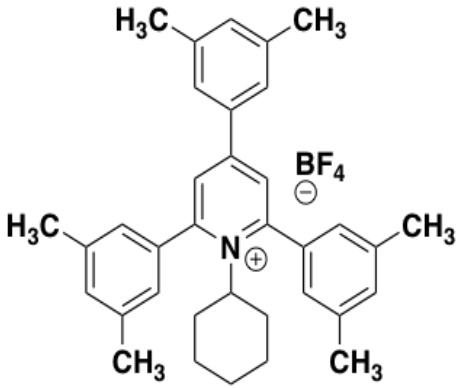

Compound **1e-Cy**

$^{19}F$ NMR (376 MHz, $CDCl_3$)



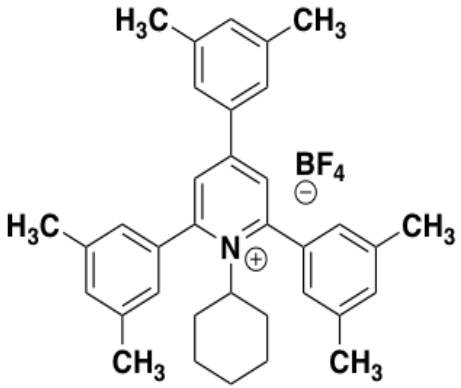

Compound **1g-Cy**

$^1$H NMR (600 MHz, $CDCl_3$)



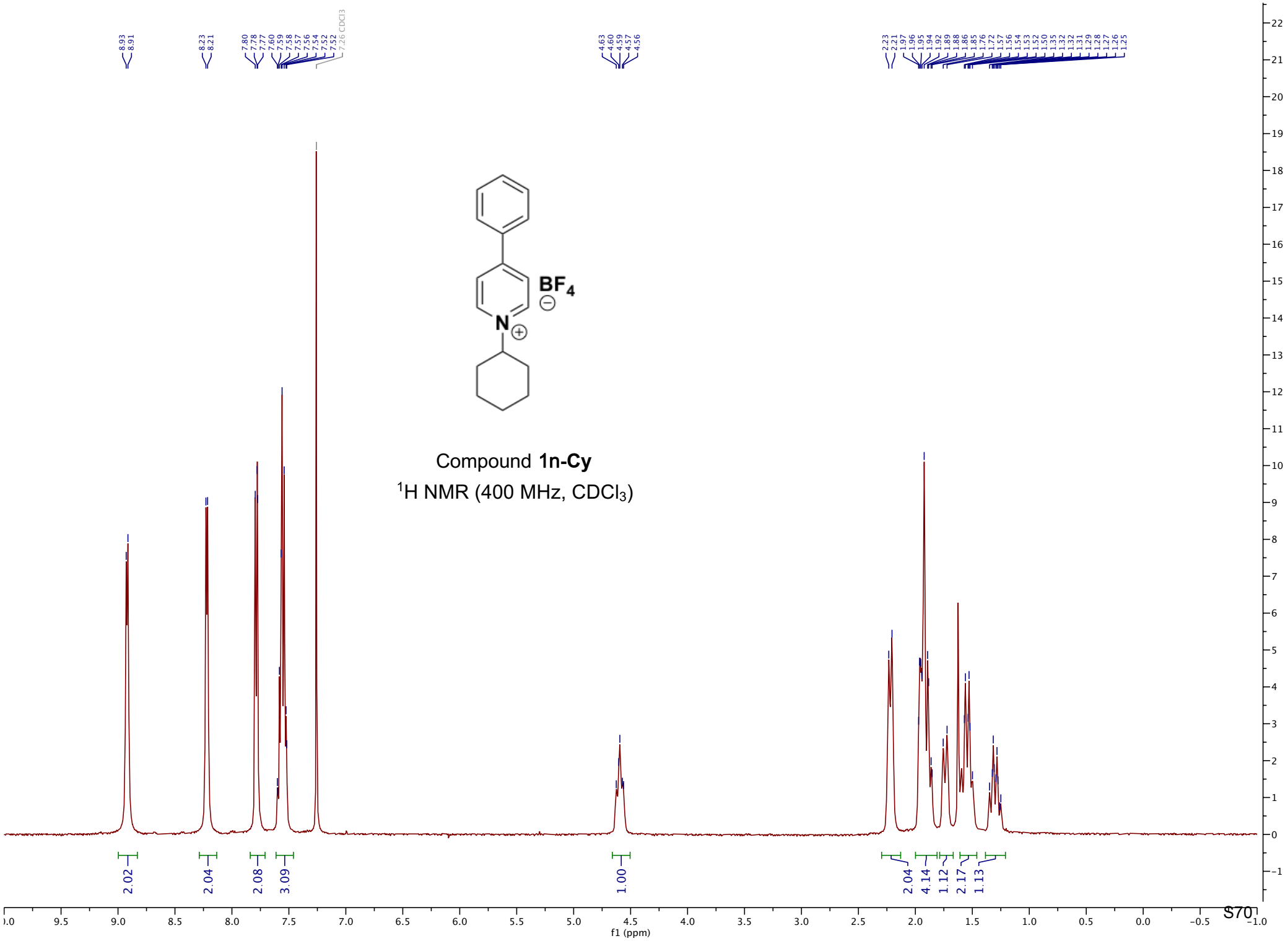

Compound **1g-Cy**

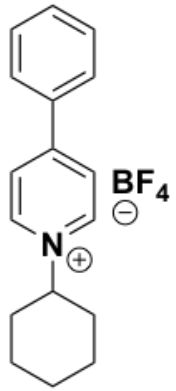
$^{13}C$ NMR (151 MHz, $CDCl_3$)




Compound **1g-Cy**

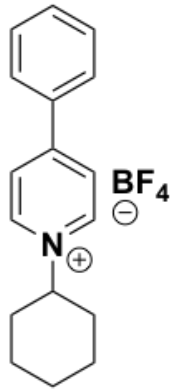
$^{19}F$ NMR (376 MHz, $CDCl_3$)


8.93
8.91
8.23
8.21
7.80
7.78
7.77
7.60
7.59
7.58
7.57
7.56
7.54
7.52
7.52
7.26 CDCl3
4.63
4.60
4.59
4.57
4.56
2.23
2.21
1.97
1.96
1.95
1.94
1.92
1.89
1.88
1.86
1.85
1.76
1.72
1.57
1.56
1.54
1.53
1.52
1.50
1.35
1.32
1.32
1.31
1.29
1.28
1.27
1.26
1.25
BF4
N
Compound 1n-Cy
1H NMR (400 MHz, CDCl3)
2.02
2.04
2.08
3.09
1.00
2.04
4.14
1.12
2.17
1.13
f1 (ppm)




Compound **1n-Cy**

$^{13}C$ NMR (101 MHz, $CDCl_3$)




Compound **1n-Cy**

$^{19}F$ NMR (376 MHz, $CDCl_3$)